



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## pH-metric Result

logP (XH2 2+) -5.50  
logP (XH +) -0.05 ±0.07 (n=50)  
logP (neutral X) 1.93 ±0.01 (n=50)

### 18C-01005 Points 1 to 35

M15\_octanol concentration factor 0.875  
Carbonate 0.2232 mM  
Acidity error -0.23667 mM

### 18C-01005 Points 36 to 71

M15\_octanol concentration factor 0.909  
Carbonate 0.1837 mM  
Acidity error -0.20987 mM

### 18C-01005 Points 72 to 105

M15\_octanol concentration factor 0.947  
Carbonate 0.0524 mM  
Acidity error -0.05926 mM

## Warnings and errors

Errors None  
Warnings One or more logP values out of range

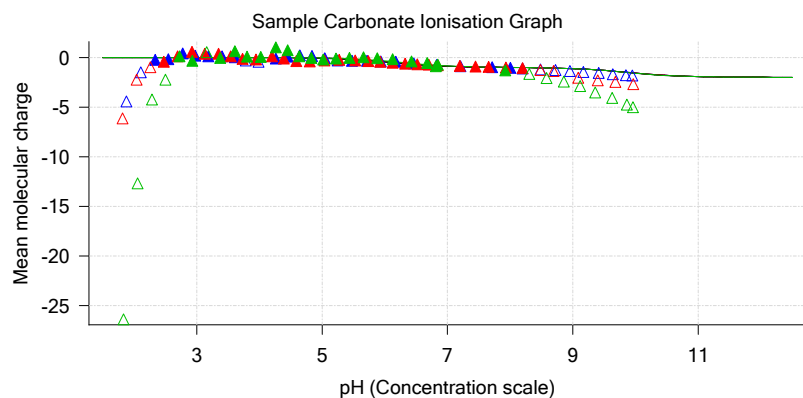
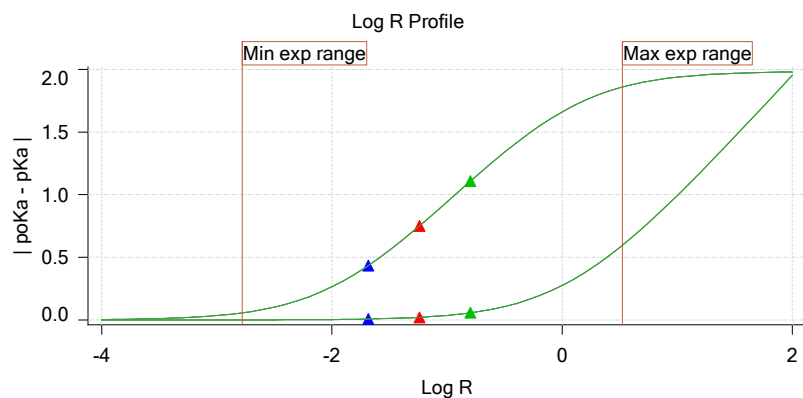
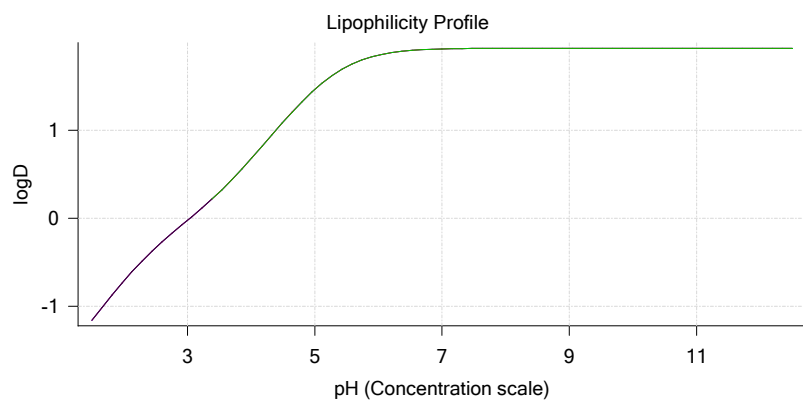
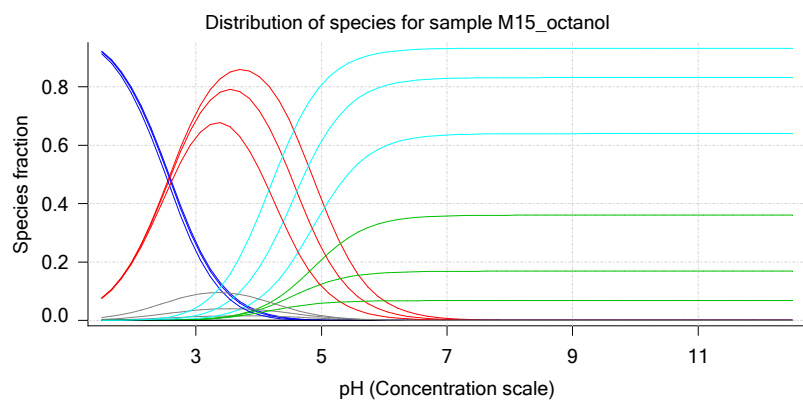
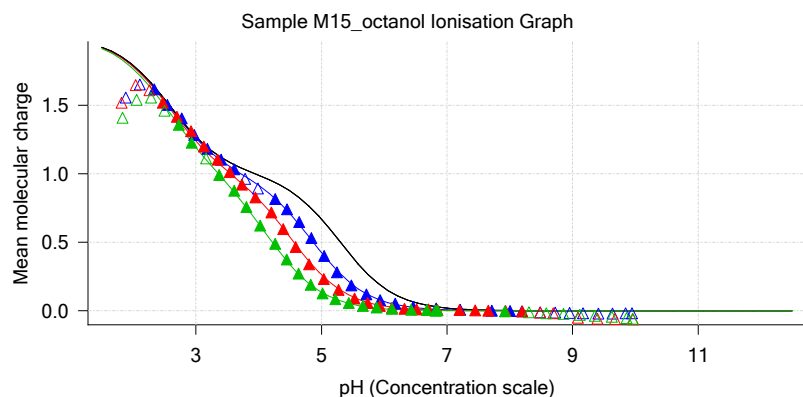
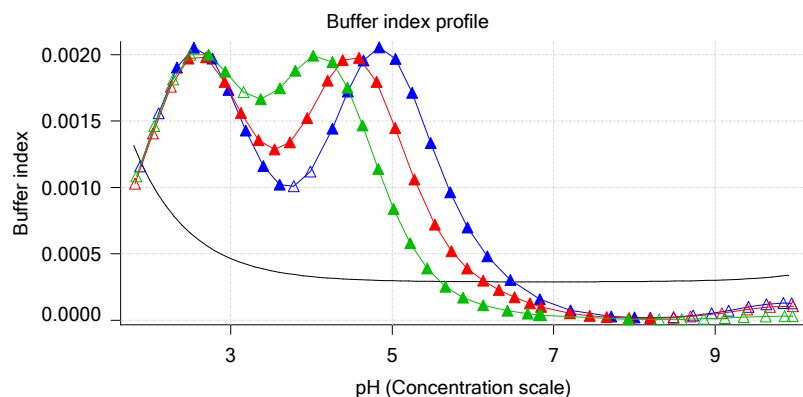
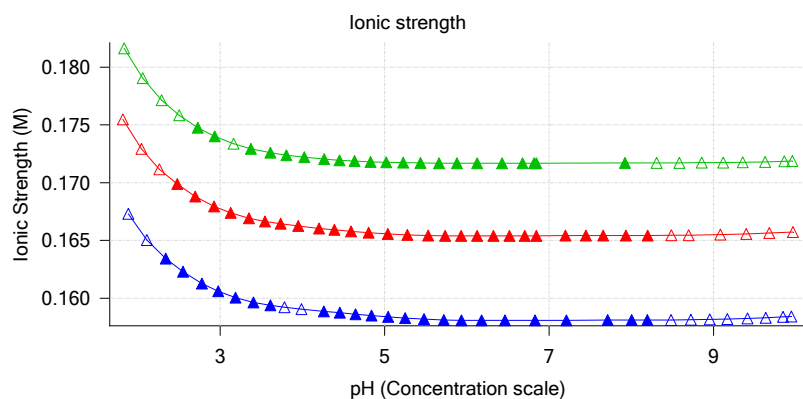
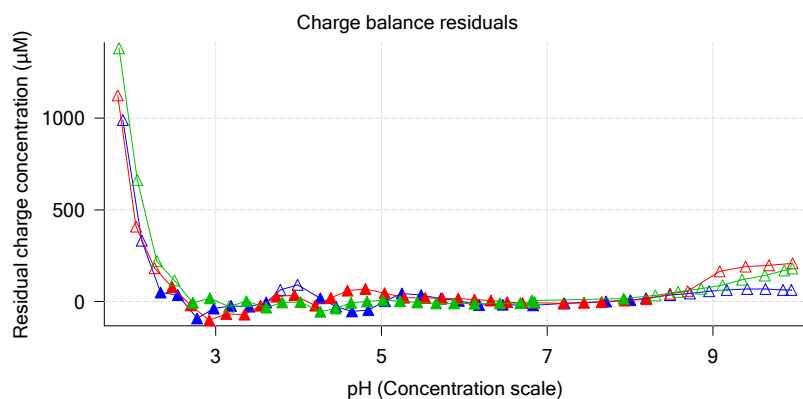
## Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-1.64	95.26 %	2.51 %	0.00 %	0.00 %	2.22 %	0.01 %	Stomach pH
1.200	-1.45	92.68 %	3.86 %	0.00 %	0.00 %	3.43 %	0.03 %	
2.000	-0.71	66.33 %	17.45 %	0.01 %	0.00 %	15.47 %	0.75 %	
3.000	-0.02	14.08 %	37.04 %	0.19 %	0.00 %	32.84 %	15.86 %	Blood pH
4.000	0.68	0.61 %	15.98 %	0.80 %	0.00 %	14.17 %	68.44 %	
5.000	1.46	0.01 %	2.21 %	1.11 %	0.00 %	1.96 %	94.71 %	
6.000	1.85	0.00 %	0.23 %	1.15 %	0.00 %	0.20 %	98.41 %	
6.500	1.91	0.00 %	0.07 %	1.16 %	0.00 %	0.06 %	98.71 %	
7.000	1.92	0.00 %	0.02 %	1.16 %	0.00 %	0.02 %	98.80 %	
7.400	1.93	0.00 %	0.01 %	1.16 %	0.00 %	0.01 %	98.83 %	
8.000	1.93	0.00 %	0.00 %	1.16 %	0.00 %	0.00 %	98.84 %	
9.000	1.93	0.00 %	0.00 %	1.16 %	0.00 %	0.00 %	98.84 %	
10.000	1.93	0.00 %	0.00 %	1.16 %	0.00 %	0.00 %	98.84 %	
11.000	1.93	0.00 %	0.00 %	1.16 %	0.00 %	0.00 %	98.84 %	
12.000	1.93	0.00 %	0.00 %	1.16 %	0.00 %	0.00 %	98.84 %	

Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

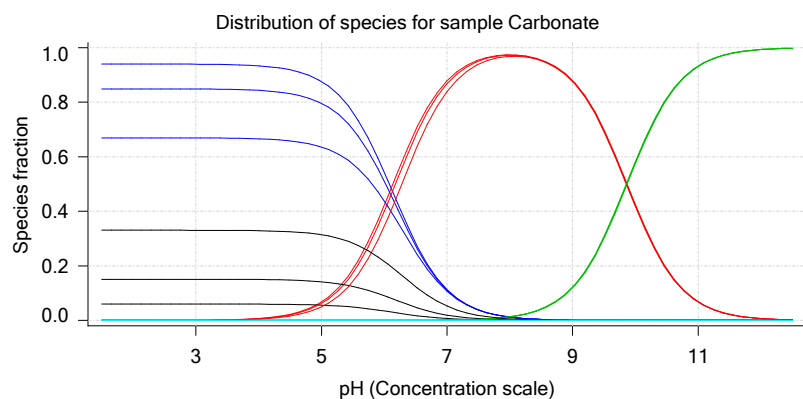
Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Graphs



Sample name: **M15\_octanol** Experiment start time: **3/1/2018 6:16:08 AM**  
 Assay name: **pH-metric high logP** Analyst: **Pion**  
 Assay ID: **18C-01005** Instrument ID: **T312060**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

## Graphs (continued)



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## pH-metric high logP Titration 1 of 3 18C-01005 Points 1 to 35

### Overall results

RMSD 0.176  
 Average ionic strength 0.159 M  
 Average temperature 25.0°C  
 Partition ratio 0.0208 : 1  
 Analyte concentration range 3855.0 µM to 4000.4 µM  
 Total points considered 23 of 35

### Warnings and errors

Errors None  
 Warnings One or more logP values out of range

### Four-Plus parameters

Alpha 0.130 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 S 0.9970 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jH 0.8 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jOH -0.4 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r

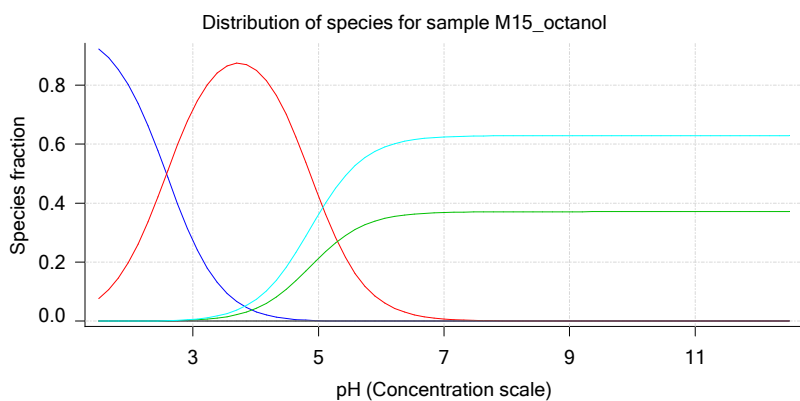
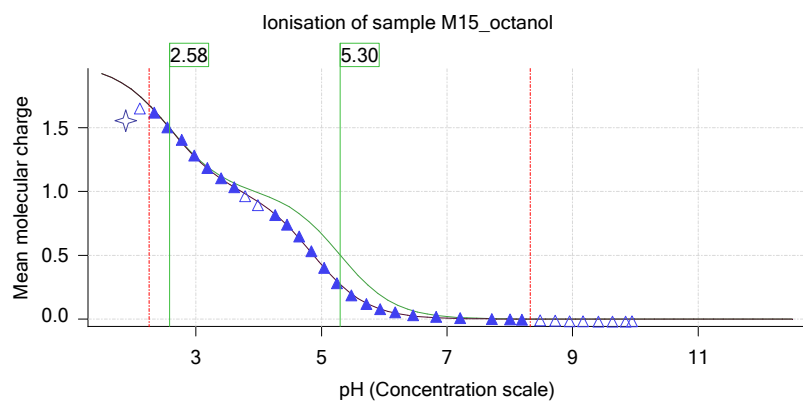
### Titrants

0.50 M HCl 0.993513 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 0.50 M KOH 0.999845 3/1/2018 6:16:08 AM C:\Sirius\_T3\KOH18B27.t3r

### Sample

M15\_octanol concentration factor 0.875  
 Base pKa 1 2.58  
 Base pKa 2 5.30  
 logP (XH2 2+) -5.50  
 logP (XH +) -3.48  
 logP (neutral X) 1.91

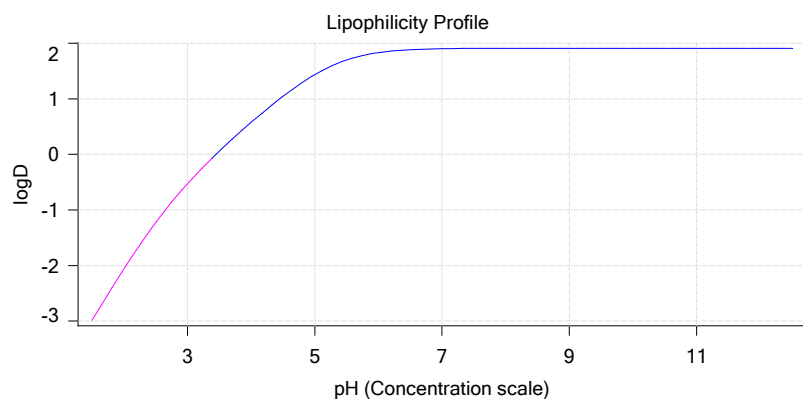
### Sample graphs



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Sample graphs (continued)



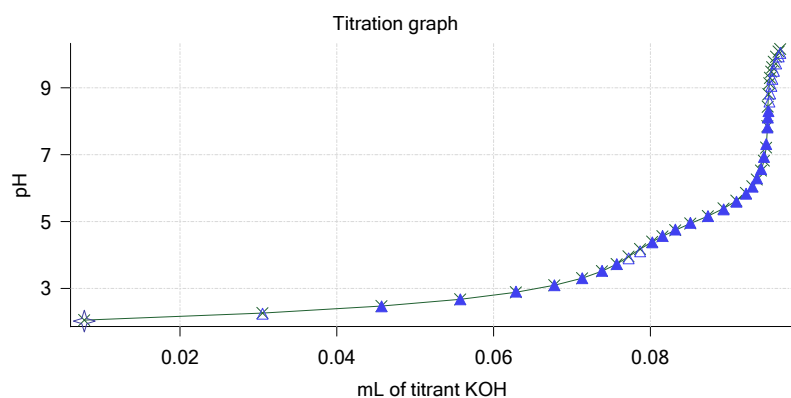
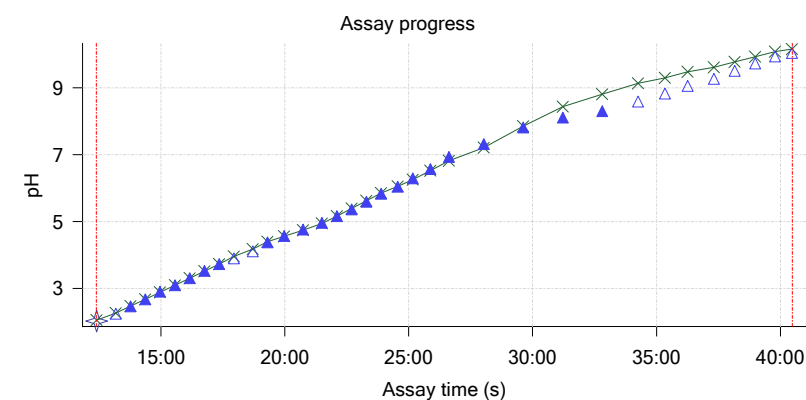
## Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.93	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
1.200	-3.56	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	
2.000	-2.07	79.15 %	20.82 %	0.01 %	0.00 %	0.00 %	0.02 %	
3.000	-0.53	27.28 %	71.75 %	0.36 %	0.00 %	0.00 %	0.61 %	
4.000	0.58	3.24 %	85.24 %	4.27 %	0.00 %	0.00 %	7.24 %	Blood pH
5.000	1.43	0.16 %	42.47 %	21.28 %	0.00 %	0.00 %	36.08 %	
6.000	1.83	0.00 %	6.89 %	34.54 %	0.00 %	0.00 %	58.56 %	
6.500	1.89	0.00 %	2.29 %	36.25 %	0.00 %	0.00 %	61.46 %	
7.000	1.90	0.00 %	0.73 %	36.83 %	0.00 %	0.00 %	62.44 %	
7.400	1.91	0.00 %	0.29 %	36.99 %	0.00 %	0.00 %	62.71 %	
8.000	1.91	0.00 %	0.07 %	37.07 %	0.00 %	0.00 %	62.85 %	
9.000	1.91	0.00 %	0.01 %	37.10 %	0.00 %	0.00 %	62.89 %	
10.000	1.91	0.00 %	0.00 %	37.10 %	0.00 %	0.00 %	62.90 %	
11.000	1.91	0.00 %	0.00 %	37.10 %	0.00 %	0.00 %	62.90 %	
12.000	1.91	0.00 %	0.00 %	37.10 %	0.00 %	0.00 %	62.90 %	

## Carbonate and acidity

Carbonate 0.223 mM  
Acidity error -0.237 mM

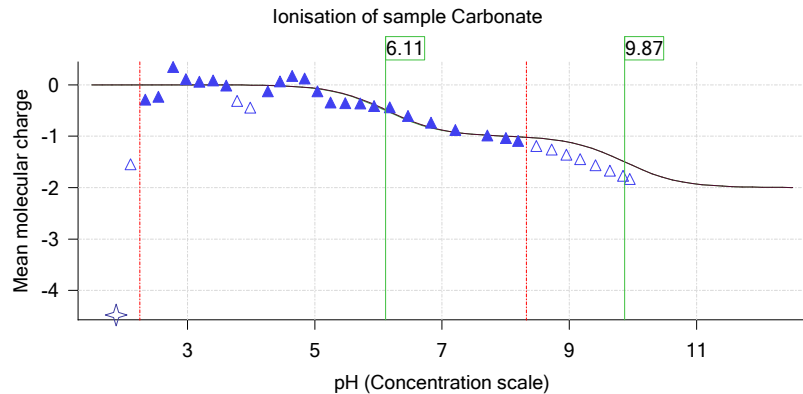
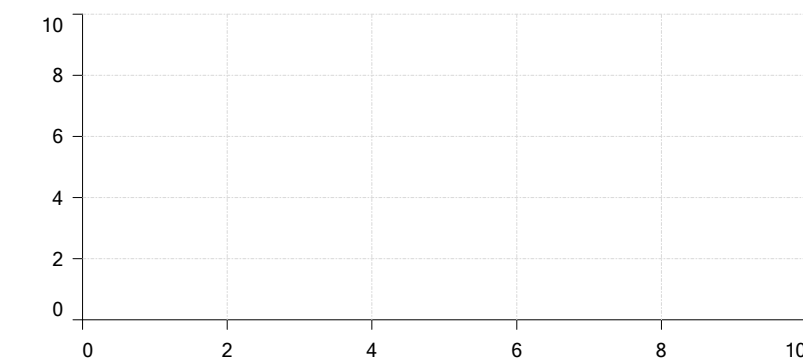
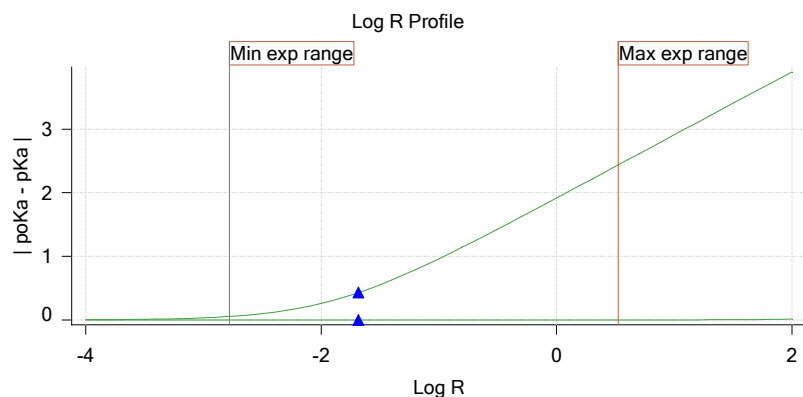
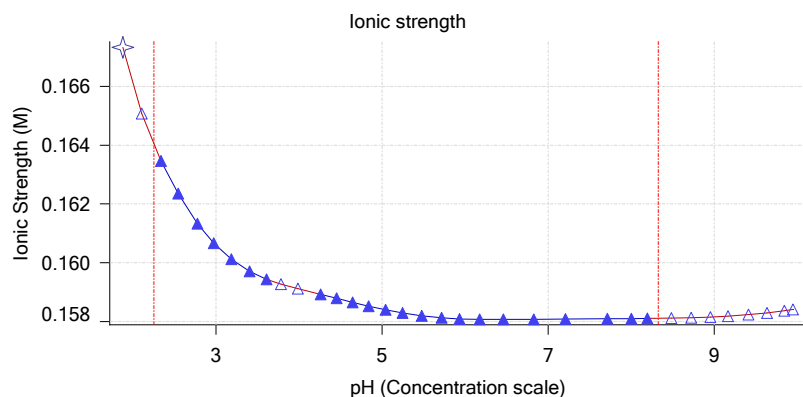
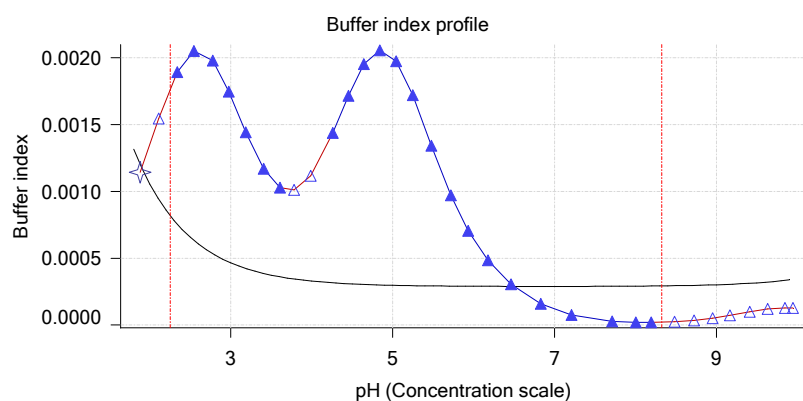
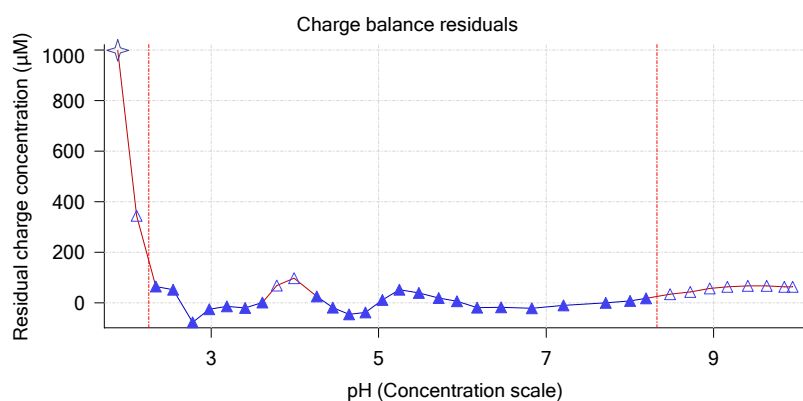
## Other graphs



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## pH-metric high logP Titration 2 of 3 18C-01005 Points 36 to 71

### Overall results

RMSD 0.148  
 Average ionic strength 0.166 M  
 Average temperature 25.0°C  
 Partition ratio 0.0576 : 1  
 Analyte concentration range 3420.0 µM to 3556.1 µM  
 Total points considered 27 of 36

### Warnings and errors

Errors None  
 Warnings One or more logP values out of range

### Four-Plus parameters

Alpha 0.130 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 S 0.9970 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jH 0.8 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jOH -0.4 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r

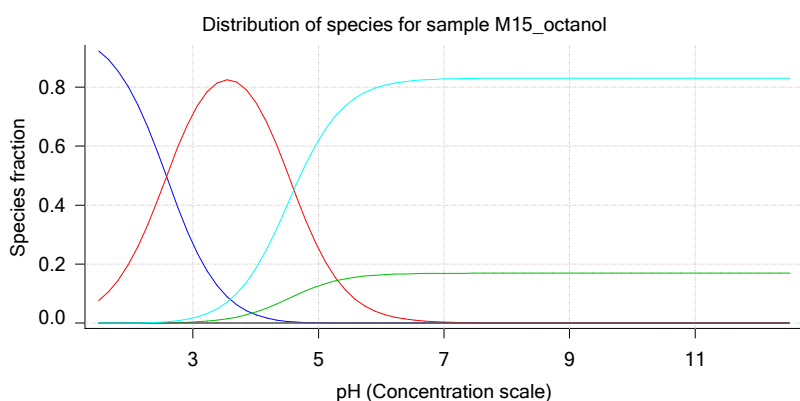
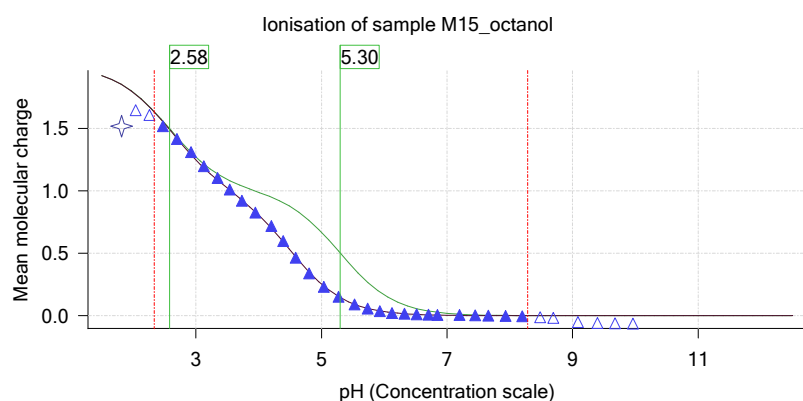
### Titrants

0.50 M HCl 0.993513 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 0.50 M KOH 0.999845 3/1/2018 6:16:08 AM C:\Sirius\_T3\KOH18B27.t3r

### Sample

M15\_octanol concentration factor 0.909  
 Base pKa 1 2.58  
 Base pKa 2 5.30  
 logP (XH2 2+) -5.50  
 logP (XH +) -4.43  
 logP (neutral X) 1.93

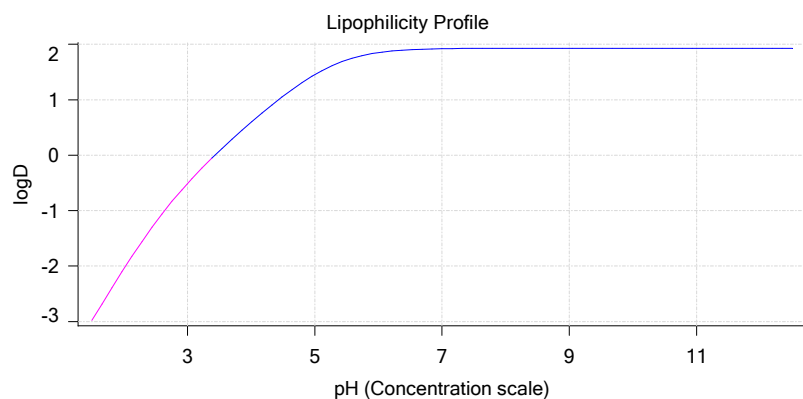
### Sample graphs



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Sample graphs (continued)



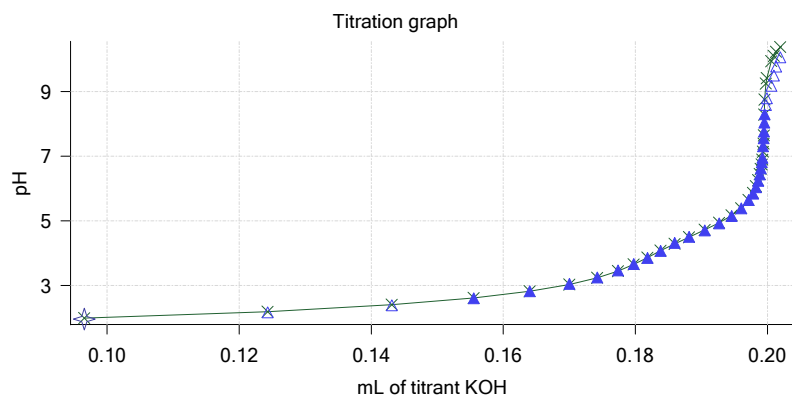
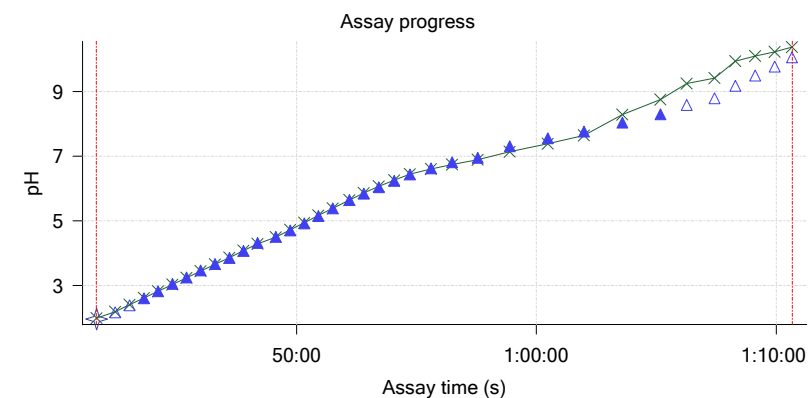
## Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.95	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
1.200	-3.56	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	
2.000	-2.05	79.13 %	20.81 %	0.01 %	0.00 %	0.00 %	0.05 %	
3.000	-0.51	26.97 %	70.93 %	0.36 %	0.00 %	0.00 %	1.74 %	Blood pH
4.000	0.59	2.85 %	74.97 %	3.76 %	0.00 %	0.00 %	18.42 %	
5.000	1.45	0.10 %	25.24 %	12.65 %	0.00 %	0.00 %	62.01 %	
6.000	1.85	0.00 %	3.27 %	16.39 %	0.00 %	0.00 %	80.34 %	
6.500	1.90	0.00 %	1.06 %	16.76 %	0.00 %	0.00 %	82.18 %	
7.000	1.92	0.00 %	0.34 %	16.89 %	0.00 %	0.00 %	82.78 %	
7.400	1.93	0.00 %	0.13 %	16.92 %	0.00 %	0.00 %	82.94 %	
8.000	1.93	0.00 %	0.03 %	16.94 %	0.00 %	0.00 %	83.03 %	
9.000	1.93	0.00 %	0.00 %	16.94 %	0.00 %	0.00 %	83.05 %	
10.000	1.93	0.00 %	0.00 %	16.94 %	0.00 %	0.00 %	83.06 %	
11.000	1.93	0.00 %	0.00 %	16.94 %	0.00 %	0.00 %	83.06 %	
12.000	1.93	0.00 %	0.00 %	16.94 %	0.00 %	0.00 %	83.06 %	

## Carbonate and acidity

Carbonate 0.184 mM  
 Acidity error -0.210 mM

## Other graphs

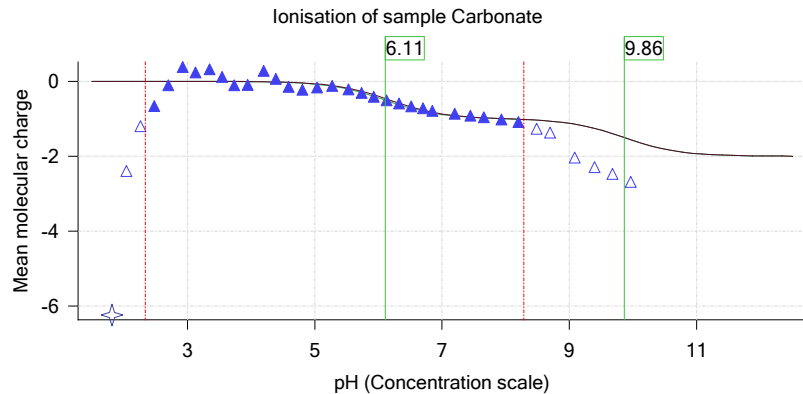
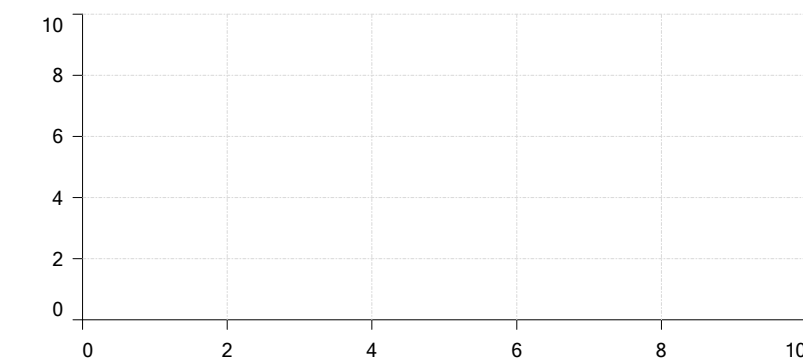
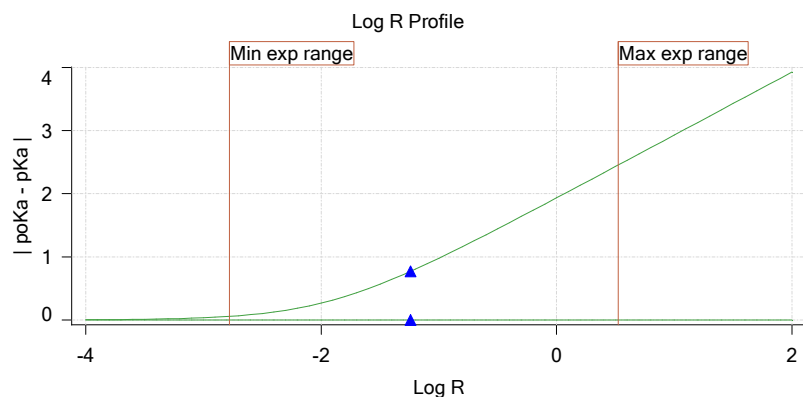
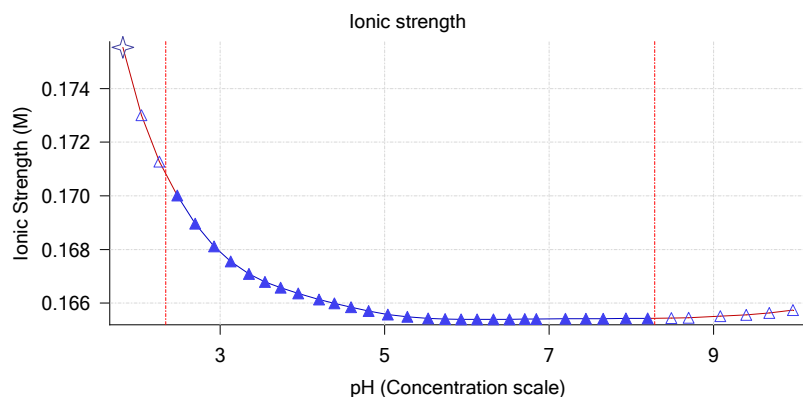
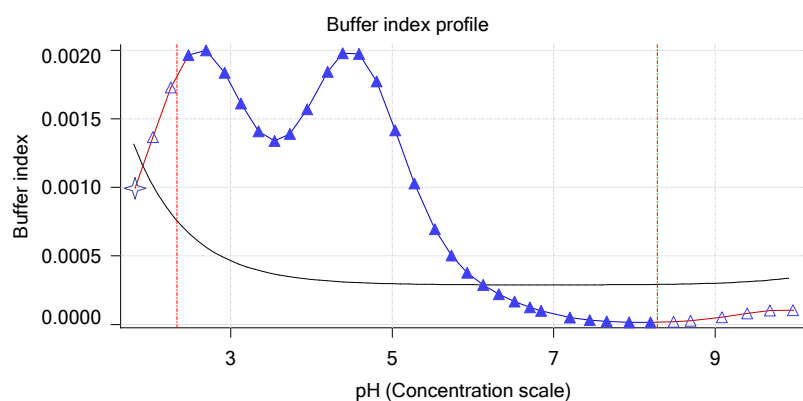
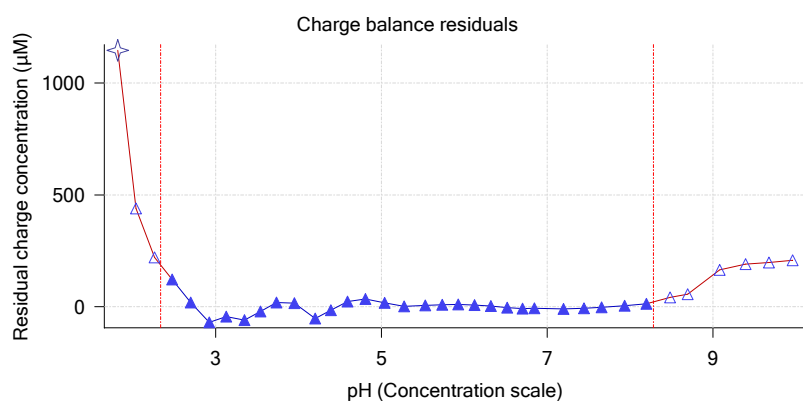




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 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-01005 Points 72 to 105

## Overall results

RMSD 0.401  
 Average ionic strength 0.172 M  
 Average temperature 25.0°C  
 Partition ratio 0.1600 : 1  
 Analyte concentration range 2881.0 µM to 2978.5 µM  
 Total points considered 21 of 34

## Warnings and errors

Errors None  
 Warnings One or more logP values out of range

## Four-Plus parameters

Alpha 0.130 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 S 0.9970 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jH 0.8 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 jOH -0.4 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r

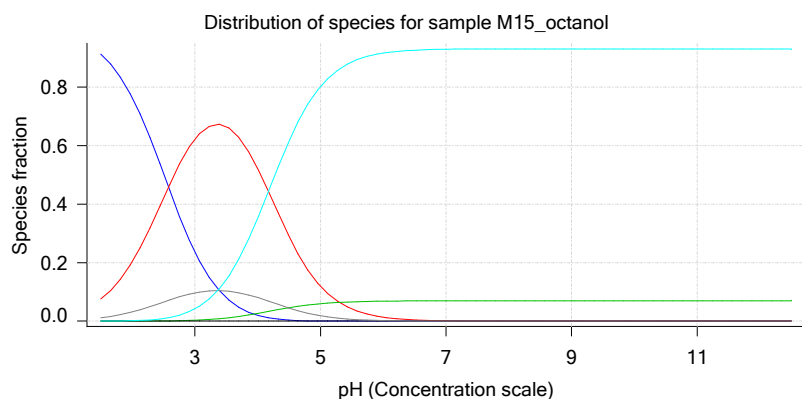
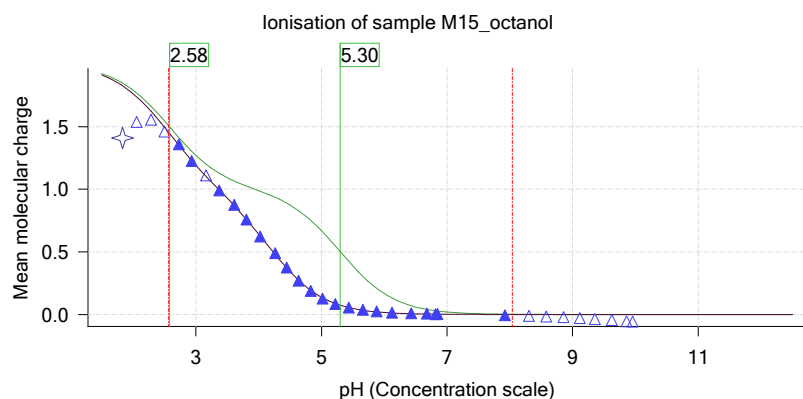
## Titrants

0.50 M HCl 0.993513 3/1/2018 6:16:08 AM C:\Sirius\_T3\HCl18B27.t3r  
 0.50 M KOH 0.999845 3/1/2018 6:16:08 AM C:\Sirius\_T3\KOH18B27.t3r

## Sample

M15\_octanol concentration factor 0.947  
 Base pKa 1 2.58  
 Base pKa 2 5.30  
 logP (XH2 2+) -5.50  
 logP (XH +) -0.01  
 logP (neutral X) 1.92

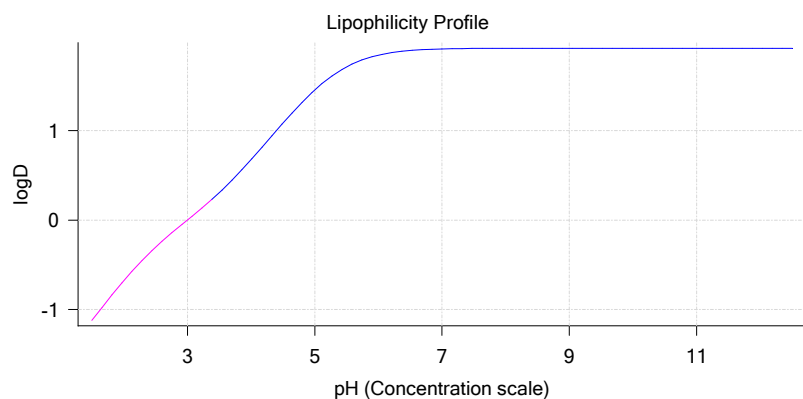
## Sample graphs



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Sample graphs (continued)



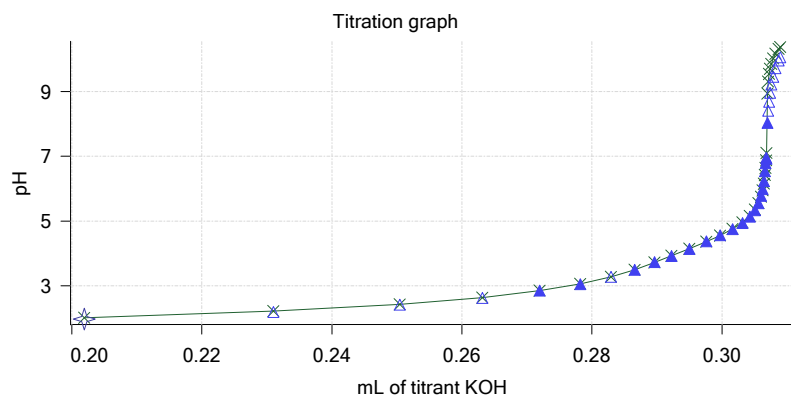
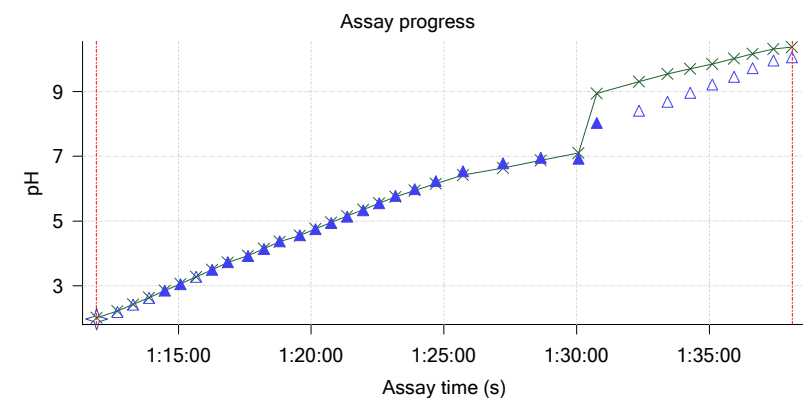
## Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-1.60	97.05 %	2.55 %	0.00 %	0.00 %	0.40 %	0.00 %	Stomach pH
1.200	-1.41	95.40 %	3.98 %	0.00 %	0.00 %	0.62 %	0.00 %	
2.000	-0.68	76.59 %	20.15 %	0.01 %	0.00 %	3.12 %	0.14 %	
3.000	0.00	23.66 %	62.22 %	0.31 %	0.00 %	9.63 %	4.18 %	Blood pH
4.000	0.68	1.99 %	52.22 %	2.62 %	0.00 %	8.08 %	35.10 %	
5.000	1.46	0.05 %	11.93 %	5.98 %	0.00 %	1.85 %	80.20 %	
6.000	1.85	0.00 %	1.36 %	6.83 %	0.00 %	0.21 %	91.60 %	
6.500	1.90	0.00 %	0.44 %	6.90 %	0.00 %	0.07 %	92.59 %	
7.000	1.91	0.00 %	0.14 %	6.93 %	0.00 %	0.02 %	92.91 %	
7.400	1.92	0.00 %	0.06 %	6.93 %	0.00 %	0.01 %	93.00 %	
8.000	1.92	0.00 %	0.01 %	6.94 %	0.00 %	0.00 %	93.05 %	
9.000	1.92	0.00 %	0.00 %	6.94 %	0.00 %	0.00 %	93.06 %	
10.000	1.92	0.00 %	0.00 %	6.94 %	0.00 %	0.00 %	93.06 %	
11.000	1.92	0.00 %	0.00 %	6.94 %	0.00 %	0.00 %	93.06 %	
12.000	1.92	0.00 %	0.00 %	6.94 %	0.00 %	0.00 %	93.06 %	

## Carbonate and acidity

Carbonate 0.052 mM  
 Acidity error -0.059 mM

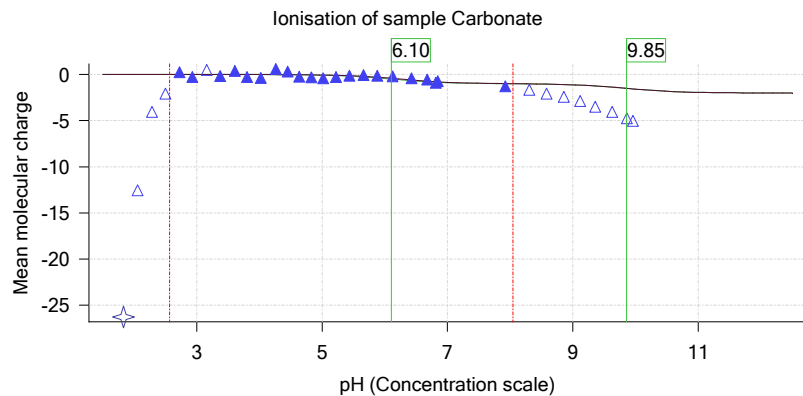
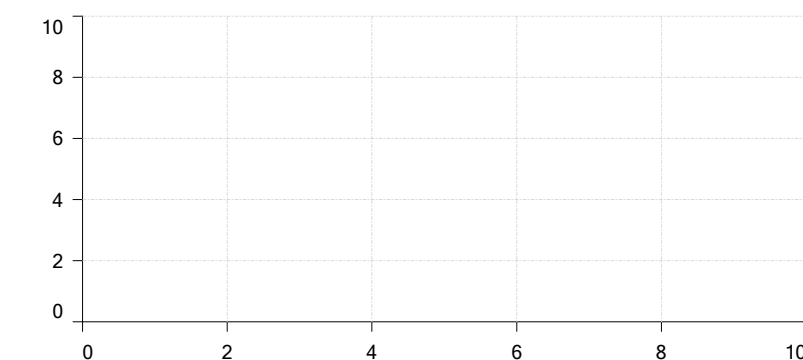
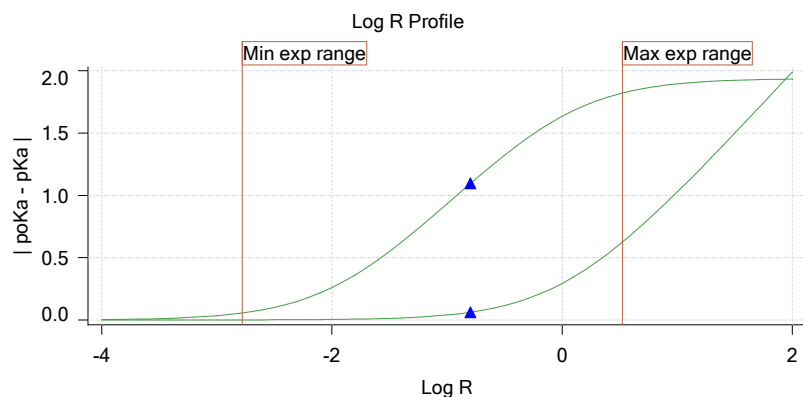
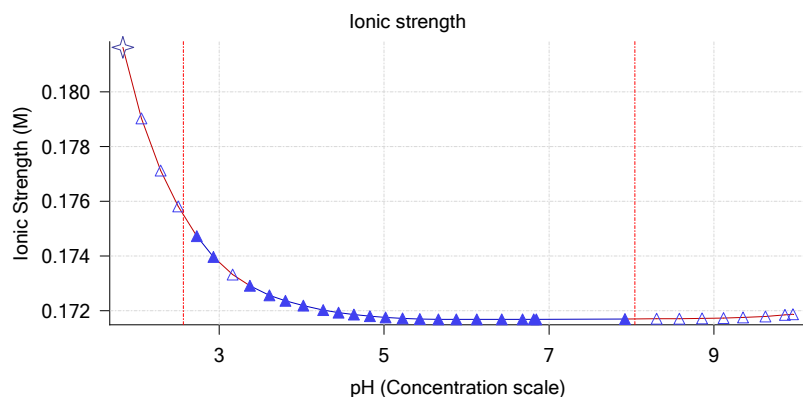
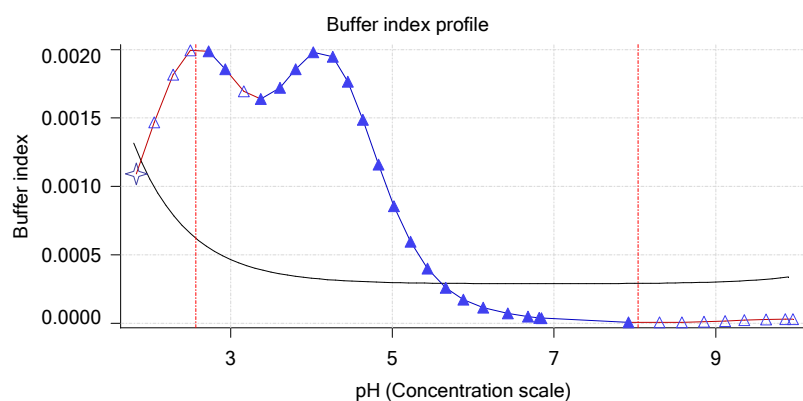
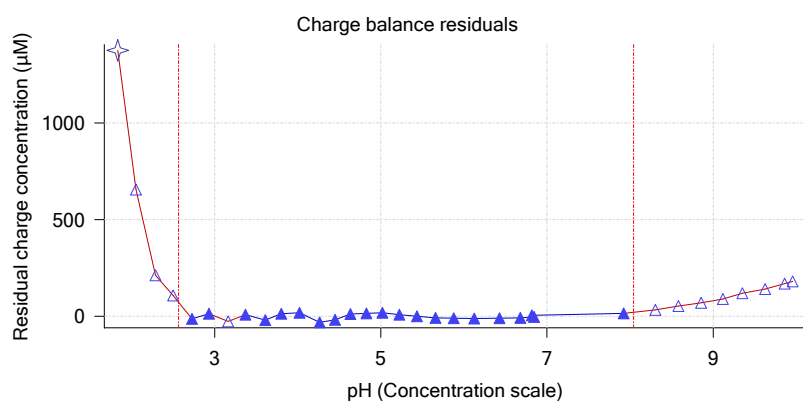
## Other graphs



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M15_octanol	2/27/2018 5:03:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001970 g	2/28/2018 4:25:24 PM	User entered value
Formula weight	209.25 g/mol	2/27/2018 5:03:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	209.25	2/27/2018 5:03:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:03:03 PM	User entered value
Sample is a	Base	2/27/2018 5:03:03 PM	User entered value
pKa 1	2.58	2/27/2018 5:03:03 PM	User entered value
pKa 2	5.30	2/27/2018 5:03:03 PM	User entered value
logP (XH2 2+)	-5.50	2/28/2018 2:10:35 PM	User entered value
logp (XH +)	-4.96	2/28/2018 2:10:28 PM	User entered value
logP (neutral X)	1.92	2/28/2018 2:10:15 PM	User entered value

## Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:23.6	Initial pH = 7.47									
12:24.5	Data point 1	2.20002 mL	0.09563 mL	0.00778 mL	0.05000 mL	2.016	0.00623	0.50576	0.00043	10.0 s
13:10.8	Data point 2	2.20002 mL	0.09563 mL	0.03050 mL	0.05000 mL	2.239	-0.00953	0.35232	0.00079	10.0 s
13:46.7	Data point 3	2.20002 mL	0.09563 mL	0.04570 mL	0.05000 mL	2.464	-0.00246	0.19027	0.00028	10.0 s
14:22.3	Data point 4	2.20002 mL	0.09563 mL	0.05576 mL	0.05000 mL	2.670	0.01234	0.53634	0.00083	10.0 s
14:58.0	Data point 5	2.20002 mL	0.09563 mL	0.06286 mL	0.05000 mL	2.900	0.00043	0.01947	0.00015	10.5 s
15:34.0	Data point 6	2.20002 mL	0.09563 mL	0.06776 mL	0.05000 mL	3.097	-0.00497	0.18772	0.00057	10.0 s
16:09.5	Data point 7	2.20002 mL	0.09563 mL	0.07131 mL	0.05000 mL	3.307	-0.00870	0.18868	0.00099	10.0 s
16:45.1	Data point 8	2.20002 mL	0.09563 mL	0.07385 mL	0.05000 mL	3.525	-0.00071	0.08489	0.00012	10.5 s
17:21.0	Data point 9	2.20002 mL	0.09563 mL	0.07571 mL	0.05000 mL	3.728	-0.00085	0.13611	0.00011	10.0 s
17:56.5	Data point 10	2.20002 mL	0.09563 mL	0.07723 mL	0.05000 mL	3.901	-0.00101	0.13288	0.00014	10.0 s
18:42.4	Data point 11	2.20002 mL	0.09563 mL	0.07869 mL	0.05000 mL	4.105	-0.00256	0.29892	0.00023	10.0 s
19:17.9	Data point 12	2.20002 mL	0.09563 mL	0.08022 mL	0.05000 mL	4.378	-0.00592	0.25762	0.00058	10.0 s
19:58.5	Data point 13	2.20002 mL	0.09563 mL	0.08154 mL	0.05000 mL	4.569	-0.00172	0.03384	0.00046	10.0 s
20:44.3	Data point 14	2.20002 mL	0.09563 mL	0.08316 mL	0.05000 mL	4.761	-0.00067	0.00810	0.00037	10.0 s
21:30.1	Data point 15	2.20002 mL	0.09563 mL	0.08511 mL	0.05000 mL	4.956	-0.00175	0.25727	0.00017	10.5 s
22:06.1	Data point 16	2.20002 mL	0.09563 mL	0.08732 mL	0.05000 mL	5.158	-0.00440	0.41157	0.00034	10.0 s
22:41.6	Data point 17	2.20002 mL	0.09563 mL	0.08935 mL	0.05000 mL	5.362	0.00350	0.06911	0.00066	10.5 s
23:17.6	Data point 18	2.20002 mL	0.09563 mL	0.09099 mL	0.05000 mL	5.592	-0.01026	0.39926	0.00080	10.0 s
23:53.0	Data point 19	2.20002 mL	0.09563 mL	0.09222 mL	0.05000 mL	5.831	-0.00232	0.01329	0.00099	10.0 s
24:33.6	Data point 20	2.20002 mL	0.09563 mL	0.09302 mL	0.05000 mL	6.046	-0.01229	0.83805	0.00066	10.5 s
25:09.5	Data point 21	2.20002 mL	0.09563 mL	0.09358 mL	0.05000 mL	6.288	-0.01579	0.76334	0.00089	12.5 s
25:52.6	Data point 22	2.20002 mL	0.09563 mL	0.09412 mL	0.05000 mL	6.573	-0.01546	0.70398	0.00091	14.5 s
26:37.6	Data point 23	2.20002 mL	0.09563 mL	0.09450 mL	0.05000 mL	6.938	-0.01891	0.87947	0.00100	48.5 s
28:01.9	Data point 24	2.20002 mL	0.09563 mL	0.09476 mL	0.05000 mL	7.316	-0.02494	0.93500	0.00127	Timed out at 59.5 s
29:37.6	Data point 25	2.20002 mL	0.09563 mL	0.09492 mL	0.05000 mL	7.818	-0.04146	0.96788	0.00208	Timed out at 59.5 s
31:13.2	Data point 26	2.20002 mL	0.09563 mL	0.09499 mL	0.05000 mL	8.108	-0.02610	0.95271	0.00132	Timed out at 59.5 s
32:48.8	Data point 27	2.20002 mL	0.09563 mL	0.09506 mL	0.05000 mL	8.299	-0.01949	0.95727	0.00098	45.5 s
34:15.2	Data point 28	2.20002 mL	0.09563 mL	0.09518 mL	0.05000 mL	8.587	-0.01701	0.74040	0.00098	24.5 s
35:20.4	Data point 29	2.20002 mL	0.09563 mL	0.09527 mL	0.05000 mL	8.827	-0.01958	0.96654	0.00098	19.5 s
36:15.6	Data point 30	2.20002 mL	0.09563 mL	0.09541 mL	0.05000 mL	9.056	-0.01834	0.92738	0.00094	28.0 s
37:19.3	Data point 31	2.20002 mL	0.09563 mL	0.09556 mL	0.05000 mL	9.269	-0.01816	0.91609	0.00094	14.5 s
38:09.5	Data point 32	2.20002 mL	0.09563 mL	0.09577 mL	0.05000 mL	9.513	-0.01968	0.96171	0.00099	14.0 s
38:59.2	Data point 33	2.20002 mL	0.09563 mL	0.09603 mL	0.05000 mL	9.735	-0.01921	0.97472	0.00096	12.5 s
39:47.4	Data point 34	2.20002 mL	0.09563 mL	0.09635 mL	0.05000 mL	9.945	-0.00595	0.27714	0.00056	10.0 s
40:27.9	Data point 35	2.20002 mL	0.09563 mL	0.09657 mL	0.05000 mL	10.046	-0.01774	0.92128	0.00091	10.0 s

Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
41:39.6	Data point 36	2.20002 mL	0.20089 mL	0.09657 mL	0.15000 mL	1.954	-0.00850	0.92951	0.00043	10.0 s
42:26.1	Data point 37	2.20002 mL	0.20089 mL	0.12434 mL	0.15000 mL	2.171	0.00527	0.50918	0.00036	10.0 s
43:02.0	Data point 38	2.20002 mL	0.20089 mL	0.14313 mL	0.15000 mL	2.389	-0.01330	0.58147	0.00086	10.0 s
43:37.7	Data point 39	2.20002 mL	0.20089 mL	0.15550 mL	0.15000 mL	2.602	-0.00134	0.03743	0.00034	10.0 s
44:13.3	Data point 40	2.20002 mL	0.20089 mL	0.16402 mL	0.15000 mL	2.821	-0.00056	0.01526	0.00022	10.0 s
44:48.9	Data point 41	2.20002 mL	0.20089 mL	0.16999 mL	0.15000 mL	3.047	0.00129	0.22583	0.00013	10.0 s
45:24.4	Data point 42	2.20002 mL	0.20089 mL	0.17420 mL	0.15000 mL	3.248	0.00052	0.05566	0.00011	10.0 s
45:59.9	Data point 43	2.20002 mL	0.20089 mL	0.17735 mL	0.15000 mL	3.468	-0.00387	0.16203	0.00047	10.0 s
46:35.4	Data point 44	2.20002 mL	0.20089 mL	0.17975 mL	0.15000 mL	3.662	-0.00150	0.13762	0.00020	10.5 s
47:11.4	Data point 45	2.20002 mL	0.20089 mL	0.18182 mL	0.15000 mL	3.852	0.00050	0.03983	0.00012	10.0 s
47:46.8	Data point 46	2.20002 mL	0.20089 mL	0.18382 mL	0.15000 mL	4.067	-0.00502	0.37193	0.00041	10.0 s
48:22.3	Data point 47	2.20002 mL	0.20089 mL	0.18594 mL	0.15000 mL	4.318	-0.00521	0.16247	0.00064	10.0 s
49:08.2	Data point 48	2.20002 mL	0.20089 mL	0.18812 mL	0.15000 mL	4.506	-0.00615	0.38511	0.00049	10.0 s
49:43.7	Data point 49	2.20002 mL	0.20089 mL	0.19048 mL	0.15000 mL	4.707	-0.00269	0.27582	0.00025	10.0 s
50:19.1	Data point 50	2.20002 mL	0.20089 mL	0.19269 mL	0.15000 mL	4.921	-0.01206	0.44085	0.00090	10.0 s
50:54.6	Data point 51	2.20002 mL	0.20089 mL	0.19457 mL	0.15000 mL	5.153	0.00999	0.53425	0.00068	10.5 s
51:30.6	Data point 52	2.20002 mL	0.20089 mL	0.19600 mL	0.15000 mL	5.389	-0.01513	0.66733	0.00091	10.5 s
52:11.7	Data point 53	2.20002 mL	0.20089 mL	0.19715 mL	0.15000 mL	5.641	-0.01166	0.35160	0.00097	11.0 s
52:48.2	Data point 54	2.20002 mL	0.20089 mL	0.19781 mL	0.15000 mL	5.848	-0.00111	0.00552	0.00073	12.0 s
53:25.6	Data point 55	2.20002 mL	0.20089 mL	0.19826 mL	0.15000 mL	6.041	-0.01512	0.65316	0.00092	13.0 s
54:04.0	Data point 56	2.20002 mL	0.20089 mL	0.19859 mL	0.15000 mL	6.237	-0.01714	0.87476	0.00091	14.0 s
54:43.4	Data point 57	2.20002 mL	0.20089 mL	0.19882 mL	0.15000 mL	6.433	-0.01867	0.91161	0.00097	27.5 s
55:36.4	Data point 58	2.20002 mL	0.20089 mL	0.19899 mL	0.15000 mL	6.627	-0.01996	0.98353	0.00099	27.0 s
56:28.8	Data point 59	2.20002 mL	0.20089 mL	0.19911 mL	0.15000 mL	6.813	-0.01534	0.97399	0.00077	39.0 s
57:33.2	Data point 60	2.20002 mL	0.20089 mL	0.19920 mL	0.15000 mL	6.955	-0.01953	0.94508	0.00099	49.0 s
58:52.9	Data point 61	2.20002 mL	0.20089 mL	0.19932 mL	0.15000 mL	7.307	-0.03681	0.97518	0.00184	Timed out at 59.5 s
1:00:28.6	Data point 62	2.20002 mL	0.20089 mL	0.19939 mL	0.15000 mL	7.553	-0.03803	0.97454	0.00190	Timed out at 59.5 s
1:01:59.1	Data point 63	2.20002 mL	0.20089 mL	0.19944 mL	0.15000 mL	7.763	-0.03211	0.96281	0.00162	Timed out at 59.5 s
1:03:34.7	Data point 64	2.20002 mL	0.20089 mL	0.19951 mL	0.15000 mL	8.039	-0.02677	0.95360	0.00135	Timed out at 59.5 s
1:05:10.3	Data point 65	2.20002 mL	0.20089 mL	0.19958 mL	0.15000 mL	8.302	-0.01665	0.74155	0.00095	24.5 s
1:06:15.7	Data point 66	2.20002 mL	0.20089 mL	0.19977 mL	0.15000 mL	8.588	-0.01458	0.68624	0.00087	29.0 s
1:07:25.6	Data point 67	2.20002 mL	0.20089 mL	0.19988 mL	0.15000 mL	8.798	-0.01709	0.86919	0.00091	16.5 s
1:08:17.8	Data point 68	2.20002 mL	0.20089 mL	0.20059 mL	0.15000 mL	9.185	-0.01489	0.69562	0.00088	14.0 s
1:09:07.5	Data point 69	2.20002 mL	0.20089 mL	0.20094 mL	0.15000 mL	9.496	-0.01158	0.36700	0.00094	18.0 s
1:09:56.1	Data point 70	2.20002 mL	0.20089 mL	0.20132 mL	0.15000 mL	9.775	-0.01160	0.42092	0.00088	12.5 s
1:10:39.2	Data point 71	2.20002 mL	0.20089 mL	0.20193 mL	0.15000 mL	10.062	-0.01596	0.67334	0.00096	10.0 s
1:11:55.5	Data point 72	2.20002 mL	0.30889 mL	0.20193 mL	0.45000 mL	1.969	0.00067	0.00237	0.00068	10.0 s
1:12:42.0	Data point 73	2.20002 mL	0.30889 mL	0.23100 mL	0.45000 mL	2.187	0.01750	0.85670	0.00093	10.0 s
1:13:17.9	Data point 74	2.20002 mL	0.30889 mL	0.25045 mL	0.45000 mL	2.416	0.01285	0.80261	0.00071	10.0 s
1:13:53.6	Data point 75	2.20002 mL	0.30889 mL	0.26312 mL	0.45000 mL	2.628	0.00730	0.64955	0.00045	10.0 s
1:14:29.3	Data point 76	2.20002 mL	0.30889 mL	0.27197 mL	0.45000 mL	2.851	0.00165	0.38392	0.00013	10.0 s
1:15:04.8	Data point 77	2.20002 mL	0.30889 mL	0.27822 mL	0.45000 mL	3.054	0.00066	0.05640	0.00014	10.0 s
1:15:40.4	Data point 78	2.20002 mL	0.30889 mL	0.28293 mL	0.45000 mL	3.283	-0.00318	0.06439	0.00062	10.0 s
1:16:15.9	Data point 79	2.20002 mL	0.30889 mL	0.28655 mL	0.45000 mL	3.492	0.00558	0.58627	0.00036	10.0 s
1:16:51.4	Data point 80	2.20002 mL	0.30889 mL	0.28961 mL	0.45000 mL	3.729	-0.00357	0.40444	0.00028	10.0 s
1:17:37.3	Data point 81	2.20002 mL	0.30889 mL	0.29222 mL	0.45000 mL	3.922	0.00000	0.00000	0.00050	10.5 s
1:18:13.3	Data point 82	2.20002 mL	0.30889 mL	0.29497 mL	0.45000 mL	4.141	-0.00271	0.20156	0.00030	10.0 s
1:18:48.8	Data point 83	2.20002 mL	0.30889 mL	0.29758 mL	0.45000 mL	4.380	-0.00694	0.22006	0.00073	10.0 s
1:19:34.6	Data point 84	2.20002 mL	0.30889 mL	0.29972 mL	0.45000 mL	4.565	0.00192	0.03274	0.00052	10.0 s
1:20:10.1	Data point 85	2.20002 mL	0.30889 mL	0.30165 mL	0.45000 mL	4.750	-0.00572	0.22132	0.00060	10.0 s
1:20:45.6	Data point 86	2.20002 mL	0.30889 mL	0.30315 mL	0.45000 mL	4.943	-0.00051	0.00238	0.00052	10.5 s
1:21:21.6	Data point 87	2.20002 mL	0.30889 mL	0.30428 mL	0.45000 mL	5.134	-0.00660	0.13315	0.00089	10.5 s
1:21:57.5	Data point 88	2.20002 mL	0.30889 mL	0.30508 mL	0.45000 mL	5.338	-0.00192	0.01187	0.00087	11.0 s



## Assay Events

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:22:33.9	Data point 89	2.20002 mL	0.30889 mL	0.30562 mL	0.45000 mL	5.547	-0.00385	0.05953	0.00078	11.5 s
1:23:10.9	Data point 90	2.20002 mL	0.30889 mL	0.30600 mL	0.45000 mL	5.773	-0.01234	0.38543	0.00098	18.0 s
1:23:54.3	Data point 91	2.20002 mL	0.30889 mL	0.30626 mL	0.45000 mL	5.990	-0.01294	0.62761	0.00081	22.0 s
1:24:41.7	Data point 92	2.20002 mL	0.30889 mL	0.30644 mL	0.45000 mL	6.237	-0.01660	0.92533	0.00085	30.5 s
1:25:42.9	Data point 93	2.20002 mL	0.30889 mL	0.30661 mL	0.45000 mL	6.538	-0.02270	0.93887	0.00116	Timed out at 59.5 s
1:27:13.4	Data point 94	2.20002 mL	0.30889 mL	0.30670 mL	0.45000 mL	6.787	-0.03247	0.95665	0.00164	Timed out at 59.5 s
1:28:38.8	Data point 95	2.20002 mL	0.30889 mL	0.30677 mL	0.45000 mL	6.955	-0.02853	0.95075	0.00145	Timed out at 59.5 s
1:30:04.2	Data point 96	2.20002 mL	0.30889 mL	0.30682 mL	0.45000 mL	6.926	-0.00738	0.28183	0.00069	10.5 s
1:30:45.2	Data point 97	2.20002 mL	0.30889 mL	0.30699 mL	0.45000 mL	8.028	-0.06462	0.99131	0.00321	Timed out at 59.5 s
1:32:20.9	Data point 98	2.20002 mL	0.30889 mL	0.30710 mL	0.45000 mL	8.410	-0.01600	0.62423	0.00100	23.5 s
1:33:25.2	Data point 99	2.20002 mL	0.30889 mL	0.30724 mL	0.45000 mL	8.685	-0.01186	0.41042	0.00092	15.5 s
1:34:16.4	Data point 100	2.20002 mL	0.30889 mL	0.30739 mL	0.45000 mL	8.958	-0.00728	0.18983	0.00082	14.5 s
1:35:06.5	Data point 101	2.20002 mL	0.30889 mL	0.30757 mL	0.45000 mL	9.218	-0.01378	0.67757	0.00083	13.0 s
1:35:55.3	Data point 102	2.20002 mL	0.30889 mL	0.30785 mL	0.45000 mL	9.455	-0.01183	0.35300	0.00098	11.5 s
1:36:37.4	Data point 103	2.20002 mL	0.30889 mL	0.30821 mL	0.45000 mL	9.725	-0.00923	0.21248	0.00099	11.5 s
1:37:24.7	Data point 104	2.20002 mL	0.30889 mL	0.30870 mL	0.45000 mL	9.960	-0.01830	0.91815	0.00094	11.0 s
1:38:06.3	Data point 105	2.20002 mL	0.30889 mL	0.30896 mL	0.45000 mL	10.057	-0.01398	0.91248	0.00072	10.5 s
1:38:25.8	Assay volumes	2.20002 mL	0.30889 mL	0.30896 mL	0.45000 mL					



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
<b>General Settings</b>				
Analyst name	Pion			
<b>Standard Experiment Settings</b>				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
<b>Advanced General Settings</b>				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
<b>Titration Pre-Dose</b>				
Titration pre-dose	None			
<b>Assay Medium</b>				
ISA water volume	2.20 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.050 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
<b>Sample Sonication</b>				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
<b>Sample Dissolution</b>				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
<b>Carbonate purge</b>				
Perform a carbonate purge	No			
<b>Temperature Control</b>				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
<b>Titration 1</b>				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
<b>Titration 2</b>				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			



Sample name: **M15\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01005**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
<b>Titration 3</b>				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
<b>Data Point Stability</b>				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

## Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 6:16:08 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 6:16:08 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 6:16:08 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 6:16:08 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 6:16:08 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 6:16:08 AM	C:\Sirius_T3\HCl18B27.t3r

## Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M15\_octanol** Experiment start time: **3/1/2018 6:16:08 AM**  
 Assay name: **pH-metric high logP** Analyst: **Pion**  
 Assay ID: **18C-01005** Instrument ID: **T312060**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titration		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.93 mV		3/1/2018 6:16:36 AM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Triton X-100 in H2O		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.4e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.1e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M15\_octanol** Experiment start time: **3/1/2018 6:16:08 AM**  
 Assay name: **pH-metric high logP** Analyst: **Pion**  
 Assay ID: **18C-01005** Instrument ID: **T312060**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

## Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

## Experiment Log

[2:49] Air gap created for Water (0.15 M KCl)  
 [2:49] Air gap created for Acid (0.5 M HCl)  
 [2:50] Air gap created for Base (0.5 M KOH)  
 [2:50] Air gap released for Water (0.15 M KCl)  
 [2:54] Titrator arm moved over Titration position  
 [2:54] Titration 1 of 3  
 [2:54] Adding initial titrants  
 [2:54] Automatically add 2.20000 mL of water  
 [3:31] Dispensed 2.200024 mL of Water (0.15 M KCl)  
 [3:35] Titrator arm moved over Drain  
 [9:16] Titrator arm moved to Titration position  
 [9:16] Argon flow rate set to 100  
 [9:16] Stirrer speed set to 10  
 [9:21] Automatically add 0.05000 mL of Octanol  
 [9:23] Dispensed 0.050000 mL of Octanol  
 [9:24] Initial pH = 7.47  
 [9:24] Iterative adjust 7.47 -> 2.00  
 [9:24] pH 7.47 -> 2.00  
 [9:27] Air gap released for Acid (0.5 M HCl)  
 [9:27] Dispensed 0.095626 mL of Acid (0.5 M HCl)  
 [9:32] Holding pH 2.00  
 [11:33] Stirrer speed set to 0  
 [11:33] Stirrer speed set to 50  
 [11:33] Iterative adjust 1.95 -> 2.00  
 [11:33] pH 1.95 -> 2.00  
 [11:33] Air gap released for Base (0.5 M KOH)  
 [11:34] Dispensed 0.007785 mL of Base (0.5 M KOH)  
 [12:25] Stirrer speed set to 0  
 [12:35] Datapoint id 1 collected  
 [12:35] Stirrer speed set to 50  
 [12:40] pH 2.03 -> 2.23  
 [12:40] Using cautious pH adjust  
 [12:40] Dispensed 0.011783 mL of Base (0.5 M KOH)  
 [12:45] Stepping pH = 2.11  
 [12:46] Dispensed 0.009196 mL of Base (0.5 M KOH)  
 [12:51] Stepping pH = 2.21  
 [12:51] Dispensed 0.001740 mL of Base (0.5 M KOH)  
 [12:56] Stepping pH = 2.23  
 [13:11] Stirrer speed set to 0  
 [13:21] Datapoint id 2 collected  
 [13:21] Charge balance equation is out by 3.7%  
 [13:21] Stirrer speed set to 50

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[13:26] pH 2.24 -> 2.44  
[13:26] Using charge balance adjust  
[13:27] Dispensed 0.015193 mL of Base (0.5 M KOH)  
[13:47] Stirrer speed set to 0  
[13:57] Datapoint id 3 collected  
[13:57] Charge balance equation is out by 9.8%  
[13:57] Stirrer speed set to 50  
[14:02] pH 2.47 -> 2.67  
[14:02] Using charge balance adjust  
[14:02] Dispensed 0.010066 mL of Base (0.5 M KOH)  
[14:22] Stirrer speed set to 0  
[14:32] Datapoint id 4 collected  
[14:32] Charge balance equation is out by 0.9%  
[14:32] Stirrer speed set to 50  
[14:38] pH 2.68 -> 2.88  
[14:38] Using charge balance adjust  
[14:38] Dispensed 0.007103 mL of Base (0.5 M KOH)  
[14:58] Stirrer speed set to 0  
[15:09] Datapoint id 5 collected  
[15:09] Charge balance equation is out by 10.7%  
[15:09] Stirrer speed set to 50  
[15:14] pH 2.91 -> 3.11  
[15:14] Using charge balance adjust  
[15:14] Dispensed 0.004892 mL of Base (0.5 M KOH)  
[15:34] Stirrer speed set to 0  
[15:44] Datapoint id 6 collected  
[15:44] Charge balance equation is out by -6.0%  
[15:44] Stirrer speed set to 50  
[15:49] pH 3.11 -> 3.31  
[15:49] Using charge balance adjust  
[15:49] Dispensed 0.003551 mL of Base (0.5 M KOH)  
[16:10] Stirrer speed set to 0  
[16:20] Datapoint id 7 collected  
[16:20] Charge balance equation is out by 0.0%  
[16:20] Stirrer speed set to 50  
[16:25] pH 3.31 -> 3.51  
[16:25] Using charge balance adjust  
[16:25] Dispensed 0.002540 mL of Base (0.5 M KOH)  
[16:45] Stirrer speed set to 0  
[16:56] Datapoint id 8 collected  
[16:56] Charge balance equation is out by 4.9%  
[16:56] Stirrer speed set to 50  
[17:01] pH 3.53 -> 3.73  
[17:01] Using charge balance adjust  
[17:01] Dispensed 0.001858 mL of Base (0.5 M KOH)  
[17:21] Stirrer speed set to 0  
[17:31] Datapoint id 9 collected  
[17:31] Charge balance equation is out by -2.1%  
[17:31] Stirrer speed set to 50  
[17:36] pH 3.74 -> 3.94  
[17:36] Using charge balance adjust  
[17:36] Dispensed 0.001529 mL of Base (0.5 M KOH)  
[17:57] Stirrer speed set to 0  
[18:07] Datapoint id 10 collected  
[18:07] Charge balance equation is out by -17.7%  
[18:07] Stirrer speed set to 50  
[18:12] pH 3.91 -> 4.11  
[18:12] Using cautious pH adjust  
[18:12] Dispensed 0.000729 mL of Base (0.5 M KOH)

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[18:17] Stepping pH = 3.99  
[18:17] Dispensed 0.000635 mL of Base (0.5 M KOH)  
[18:22] Stepping pH = 4.09  
[18:22] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[18:27] Stepping pH = 4.11  
[18:43] Stirrer speed set to 0  
[18:53] Datapoint id 11 collected  
[18:53] Charge balance equation is out by -0.4%  
[18:53] Stirrer speed set to 50  
[18:58] pH 4.11 -> 4.31  
[18:58] Using charge balance adjust  
[18:58] Dispensed 0.001529 mL of Base (0.5 M KOH)  
[19:18] Stirrer speed set to 0  
[19:28] Datapoint id 12 collected  
[19:28] Charge balance equation is out by 33.2%  
[19:28] Stirrer speed set to 50  
[19:33] pH 4.38 -> 4.58  
[19:33] Using cautious pH adjust  
[19:33] Dispensed 0.000917 mL of Base (0.5 M KOH)  
[19:38] Stepping pH = 4.51  
[19:38] Dispensed 0.000400 mL of Base (0.5 M KOH)  
[19:44] Stepping pH = 4.57  
[19:59] Stirrer speed set to 0  
[20:09] Datapoint id 13 collected  
[20:09] Charge balance equation is out by 28.2%  
[20:09] Stirrer speed set to 50  
[20:14] pH 4.57 -> 4.77  
[20:14] Using cautious pH adjust  
[20:14] Dispensed 0.001035 mL of Base (0.5 M KOH)  
[20:19] Stepping pH = 4.70  
[20:19] Dispensed 0.000494 mL of Base (0.5 M KOH)  
[20:24] Stepping pH = 4.76  
[20:24] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[20:29] Stepping pH = 4.77  
[20:44] Stirrer speed set to 0  
[20:54] Datapoint id 14 collected  
[20:54] Charge balance equation is out by 22.3%  
[20:54] Stirrer speed set to 50  
[21:00] pH 4.77 -> 4.97  
[21:00] Using cautious pH adjust  
[21:00] Dispensed 0.001129 mL of Base (0.5 M KOH)  
[21:05] Stepping pH = 4.88  
[21:05] Dispensed 0.000635 mL of Base (0.5 M KOH)  
[21:10] Stepping pH = 4.95  
[21:10] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[21:15] Stepping pH = 4.96  
[21:30] Stirrer speed set to 0  
[21:41] Datapoint id 15 collected  
[21:41] Charge balance equation is out by 12.8%  
[21:41] Stirrer speed set to 50  
[21:46] pH 4.96 -> 5.16  
[21:46] Using charge balance adjust  
[21:46] Dispensed 0.002211 mL of Base (0.5 M KOH)  
[22:06] Stirrer speed set to 0  
[22:16] Datapoint id 16 collected  
[22:16] Charge balance equation is out by -2.8%  
[22:16] Stirrer speed set to 50  
[22:21] pH 5.16 -> 5.36  
[22:21] Using charge balance adjust

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[22:22] Dispensed 0.002023 mL of Base (0.5 M KOH)  
[22:42] Stirrer speed set to 0  
[22:52] Datapoint id 17 collected  
[22:52] Charge balance equation is out by -0.1%  
[22:52] Stirrer speed set to 50  
[22:57] pH 5.37 -> 5.57  
[22:57] Using charge balance adjust  
[22:57] Dispensed 0.001646 mL of Base (0.5 M KOH)  
[23:18] Stirrer speed set to 0  
[23:28] Datapoint id 18 collected  
[23:28] Charge balance equation is out by 12.1%  
[23:28] Stirrer speed set to 50  
[23:33] pH 5.60 -> 5.80  
[23:33] Using charge balance adjust  
[23:33] Dispensed 0.001223 mL of Base (0.5 M KOH)  
[23:53] Stirrer speed set to 0  
[24:03] Datapoint id 19 collected  
[24:03] Charge balance equation is out by 16.5%  
[24:03] Stirrer speed set to 50  
[24:08] pH 5.84 -> 6.04  
[24:08] Using cautious pH adjust  
[24:08] Dispensed 0.000423 mL of Base (0.5 M KOH)  
[24:13] Stepping pH = 5.92  
[24:14] Dispensed 0.000376 mL of Base (0.5 M KOH)  
[24:19] Stepping pH = 6.03  
[24:34] Stirrer speed set to 0  
[24:44] Datapoint id 20 collected  
[24:44] Charge balance equation is out by 3.8%  
[24:44] Stirrer speed set to 50  
[24:49] pH 6.05 -> 6.25  
[24:49] Using charge balance adjust  
[24:49] Dispensed 0.000564 mL of Base (0.5 M KOH)  
[25:10] Stirrer speed set to 0  
[25:22] Datapoint id 21 collected  
[25:22] Charge balance equation is out by 16.9%  
[25:22] Stirrer speed set to 50  
[25:27] pH 6.29 -> 6.49  
[25:27] Using cautious pH adjust  
[25:27] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[25:32] Stepping pH = 6.33  
[25:33] Dispensed 0.000353 mL of Base (0.5 M KOH)  
[25:38] Stepping pH = 6.52  
[25:53] Stirrer speed set to 0  
[26:07] Datapoint id 22 collected  
[26:07] Charge balance equation is out by -49.2%  
[26:07] Stirrer speed set to 50  
[26:12] pH 6.58 -> 6.78  
[26:12] Using cautious pH adjust  
[26:12] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[26:17] Stepping pH = 6.60  
[26:18] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[26:23] Stepping pH = 6.84  
[26:38] Stirrer speed set to 0  
[27:26] Datapoint id 23 collected  
[27:26] Charge balance equation is out by -83.4%  
[27:26] Stirrer speed set to 50  
[27:31] pH 6.94 -> 7.14  
[27:31] Using cautious pH adjust  
[27:32] Dispensed 0.000047 mL of Base (0.5 M KOH)



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[27:37] Stepping pH = 6.96  
[27:37] Dispensed 0.000118 mL of Base (0.5 M KOH)  
[27:42] Stepping pH = 7.04  
[27:42] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[27:47] Stepping pH = 7.24  
[28:02] Stirrer speed set to 0  
[29:02] Datapoint id 24 collected  
[29:02] Charge balance equation is out by -171.1%  
[29:02] Stirrer speed set to 50  
[29:07] pH 7.30 -> 7.50  
[29:07] Using cautious pH adjust  
[29:07] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[29:12] Stepping pH = 7.32  
[29:12] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[29:17] Stepping pH = 7.36  
[29:17] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[29:23] Stepping pH = 7.64  
[29:38] Stirrer speed set to 0  
[30:38] Datapoint id 25 collected  
[30:38] Charge balance equation is out by -247.2%  
[30:38] Stirrer speed set to 50  
[30:43] pH 7.80 -> 8.00  
[30:43] Using cautious pH adjust  
[30:43] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[30:48] Stepping pH = 7.88  
[30:48] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[30:53] Stepping pH = 7.97  
[30:53] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[30:58] Stepping pH = 8.09  
[31:13] Stirrer speed set to 0  
[32:13] Datapoint id 26 collected  
[32:13] Charge balance equation is out by -210.8%  
[32:13] Stirrer speed set to 50  
[32:18] pH 8.06 -> 8.26  
[32:18] Using cautious pH adjust  
[32:19] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[32:24] Stepping pH = 8.11  
[32:24] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[32:29] Stepping pH = 8.16  
[32:29] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[32:34] Stepping pH = 8.26  
[32:49] Stirrer speed set to 0  
[33:35] Datapoint id 27 collected  
[33:35] Charge balance equation is out by -276.2%  
[33:35] Stirrer speed set to 50  
[33:40] pH 8.28 -> 8.48  
[33:40] Using cautious pH adjust  
[33:40] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[33:45] Stepping pH = 8.29  
[33:45] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[33:50] Stepping pH = 8.33  
[33:50] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[33:55] Stepping pH = 8.43  
[33:55] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[34:00] Stepping pH = 8.55  
[34:15] Stirrer speed set to 0  
[34:40] Datapoint id 28 collected  
[34:40] Charge balance equation is out by -522.0%  
[34:40] Stirrer speed set to 50

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[34:45] pH 8.59 -> 8.79  
[34:45] Using cautious pH adjust  
[34:45] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[34:50] Stepping pH = 8.63  
[34:50] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[34:55] Stepping pH = 8.69  
[34:55] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[35:00] Stepping pH = 8.75  
[35:00] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[35:05] Stepping pH = 8.81  
[35:21] Stirrer speed set to 0  
[35:40] Datapoint id 29 collected  
[35:40] Charge balance equation is out by -241.0%  
[35:40] Stirrer speed set to 50  
[35:45] pH 8.84 -> 9.04  
[35:45] Using cautious pH adjust  
[35:45] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[35:50] Stepping pH = 8.86  
[35:50] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[35:55] Stepping pH = 8.93  
[35:56] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[36:01] Stepping pH = 9.03  
[36:16] Stirrer speed set to 0  
[36:44] Datapoint id 30 collected  
[36:44] Charge balance equation is out by -213.1%  
[36:44] Stirrer speed set to 50  
[36:49] pH 9.07 -> 9.27  
[36:49] Using cautious pH adjust  
[36:49] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[36:54] Stepping pH = 9.11  
[36:54] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[36:59] Stepping pH = 9.21  
[36:59] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[37:04] Stepping pH = 9.27  
[37:19] Stirrer speed set to 0  
[37:34] Datapoint id 31 collected  
[37:34] Charge balance equation is out by -90.2%  
[37:34] Stirrer speed set to 50  
[37:39] pH 9.28 -> 9.48  
[37:39] Using cautious pH adjust  
[37:39] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[37:44] Stepping pH = 9.31  
[37:44] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[37:49] Stepping pH = 9.46  
[37:49] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[37:55] Stepping pH = 9.51  
[38:10] Stirrer speed set to 0  
[38:24] Datapoint id 32 collected  
[38:24] Charge balance equation is out by -88.1%  
[38:24] Stirrer speed set to 50  
[38:29] pH 9.52 -> 9.72  
[38:29] Using cautious pH adjust  
[38:29] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[38:34] Stepping pH = 9.57  
[38:34] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[38:39] Stepping pH = 9.70  
[38:39] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[38:44] Stepping pH = 9.73  
[38:59] Stirrer speed set to 0



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[39:12] Datapoint id 33 collected  
[39:12] Charge balance equation is out by -50.1%  
[39:12] Stirrer speed set to 50  
[39:17] pH 9.74 -> 9.94  
[39:17] Using cautious pH adjust  
[39:17] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[39:22] Stepping pH = 9.82  
[39:22] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[39:27] Stepping pH = 9.91  
[39:27] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[39:32] Stepping pH = 9.94  
[39:48] Stirrer speed set to 0  
[39:58] Datapoint id 34 collected  
[39:58] Charge balance equation is out by -18.1%  
[39:58] Stirrer speed set to 50  
[40:03] pH 9.95 -> 10.05  
[40:03] Using cautious pH adjust  
[40:03] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[40:08] Stepping pH = 9.98  
[40:08] Dispensed 0.000118 mL of Base (0.5 M KOH)  
[40:13] Stepping pH = 10.04  
[40:28] Stirrer speed set to 0  
[40:38] Datapoint id 35 collected  
[40:38] Charge balance equation is out by -23.6%  
[40:38] Titration 2 of 3  
[40:38] Adding initial titrants  
[40:38] Automatically add 0.10000 mL of Octanol  
[40:41] Dispensed 0.100000 mL of Octanol  
[40:41] Stirrer speed set to 10  
[40:42] Stirrer speed set to 55  
[40:42] Iterative adjust 10.05 -> 2.00  
[40:42] pH 10.05 -> 2.00  
[40:44] Dispensed 0.100000 mL of Acid (0.5 M HCl)  
[40:49] pH 2.03 -> 2.00  
[40:49] Dispensed 0.005268 mL of Acid (0.5 M HCl)  
[41:40] Stirrer speed set to 0  
[41:50] Datapoint id 36 collected  
[41:50] Stirrer speed set to 55  
[41:55] pH 1.96 -> 2.16  
[41:55] Using cautious pH adjust  
[41:55] Dispensed 0.014722 mL of Base (0.5 M KOH)  
[42:00] Stepping pH = 2.05  
[42:01] Dispensed 0.011054 mL of Base (0.5 M KOH)  
[42:06] Stepping pH = 2.14  
[42:06] Dispensed 0.001999 mL of Base (0.5 M KOH)  
[42:11] Stepping pH = 2.17  
[42:26] Stirrer speed set to 0  
[42:36] Datapoint id 37 collected  
[42:36] Charge balance equation is out by 5.8%  
[42:36] Stirrer speed set to 55  
[42:41] pH 2.17 -> 2.37  
[42:41] Using charge balance adjust  
[42:42] Dispensed 0.018791 mL of Base (0.5 M KOH)  
[43:02] Stirrer speed set to 0  
[43:12] Datapoint id 38 collected  
[43:12] Charge balance equation is out by 6.9%  
[43:12] Stirrer speed set to 55  
[43:17] pH 2.39 -> 2.59  
[43:17] Using charge balance adjust

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[43:18] Dispensed 0.012371 mL of Base (0.5 M KOH)  
[43:38] Stirrer speed set to 0  
[43:48] Datapoint id 39 collected  
[43:48] Charge balance equation is out by 4.3%  
[43:48] Stirrer speed set to 55  
[43:53] pH 2.61 -> 2.81  
[43:53] Using charge balance adjust  
[43:53] Dispensed 0.008514 mL of Base (0.5 M KOH)  
[44:13] Stirrer speed set to 0  
[44:23] Datapoint id 40 collected  
[44:23] Charge balance equation is out by 6.2%  
[44:23] Stirrer speed set to 55  
[44:29] pH 2.83 -> 3.03  
[44:29] Using charge balance adjust  
[44:29] Dispensed 0.005974 mL of Base (0.5 M KOH)  
[44:49] Stirrer speed set to 0  
[44:59] Datapoint id 41 collected  
[44:59] Charge balance equation is out by 9.4%  
[44:59] Stirrer speed set to 55  
[45:04] pH 3.05 -> 3.25  
[45:04] Using charge balance adjust  
[45:04] Dispensed 0.004210 mL of Base (0.5 M KOH)  
[45:25] Stirrer speed set to 0  
[45:35] Datapoint id 42 collected  
[45:35] Charge balance equation is out by -1.8%  
[45:35] Stirrer speed set to 55  
[45:40] pH 3.25 -> 3.45  
[45:40] Using charge balance adjust  
[45:40] Dispensed 0.003151 mL of Base (0.5 M KOH)  
[46:00] Stirrer speed set to 0  
[46:10] Datapoint id 43 collected  
[46:10] Charge balance equation is out by 8.8%  
[46:10] Stirrer speed set to 55  
[46:15] pH 3.47 -> 3.67  
[46:15] Using charge balance adjust  
[46:15] Dispensed 0.002399 mL of Base (0.5 M KOH)  
[46:36] Stirrer speed set to 0  
[46:46] Datapoint id 44 collected  
[46:46] Charge balance equation is out by -5.2%  
[46:46] Stirrer speed set to 55  
[46:51] pH 3.67 -> 3.87  
[46:51] Using charge balance adjust  
[46:51] Dispensed 0.002070 mL of Base (0.5 M KOH)  
[47:11] Stirrer speed set to 0  
[47:22] Datapoint id 45 collected  
[47:22] Charge balance equation is out by -7.7%  
[47:22] Stirrer speed set to 55  
[47:27] pH 3.86 -> 4.06  
[47:27] Using charge balance adjust  
[47:27] Dispensed 0.001999 mL of Base (0.5 M KOH)  
[47:47] Stirrer speed set to 0  
[47:57] Datapoint id 46 collected  
[47:57] Charge balance equation is out by 5.7%  
[47:57] Stirrer speed set to 55  
[48:02] pH 4.07 -> 4.27  
[48:02] Using charge balance adjust  
[48:02] Dispensed 0.002117 mL of Base (0.5 M KOH)  
[48:22] Stirrer speed set to 0  
[48:32] Datapoint id 47 collected

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[48:32] Charge balance equation is out by 24.4%  
[48:32] Stirrer speed set to 55  
[48:38] pH 4.31 -> 4.51  
[48:38] Using cautious pH adjust  
[48:38] Dispensed 0.001152 mL of Base (0.5 M KOH)  
[48:43] Stepping pH = 4.41  
[48:43] Dispensed 0.000870 mL of Base (0.5 M KOH)  
[48:48] Stepping pH = 4.50  
[48:48] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[48:53] Stepping pH = 4.51  
[49:08] Stirrer speed set to 0  
[49:18] Datapoint id 48 collected  
[49:18] Charge balance equation is out by 5.4%  
[49:18] Stirrer speed set to 55  
[49:23] pH 4.51 -> 4.71  
[49:23] Using charge balance adjust  
[49:24] Dispensed 0.002352 mL of Base (0.5 M KOH)  
[49:44] Stirrer speed set to 0  
[49:54] Datapoint id 49 collected  
[49:54] Charge balance equation is out by -0.6%  
[49:54] Stirrer speed set to 55  
[49:59] pH 4.71 -> 4.91  
[49:59] Using charge balance adjust  
[49:59] Dispensed 0.002211 mL of Base (0.5 M KOH)  
[50:19] Stirrer speed set to 0  
[50:29] Datapoint id 50 collected  
[50:29] Charge balance equation is out by 5.6%  
[50:29] Stirrer speed set to 55  
[50:34] pH 4.93 -> 5.13  
[50:34] Using charge balance adjust  
[50:35] Dispensed 0.001881 mL of Base (0.5 M KOH)  
[50:55] Stirrer speed set to 0  
[51:05] Datapoint id 51 collected  
[51:05] Charge balance equation is out by 13.1%  
[51:05] Stirrer speed set to 55  
[51:10] pH 5.16 -> 5.36  
[51:10] Using charge balance adjust  
[51:11] Dispensed 0.001435 mL of Base (0.5 M KOH)  
[51:31] Stirrer speed set to 0  
[51:41] Datapoint id 52 collected  
[51:41] Charge balance equation is out by 15.8%  
[51:41] Stirrer speed set to 55  
[51:46] pH 5.39 -> 5.59  
[51:46] Using cautious pH adjust  
[51:46] Dispensed 0.000517 mL of Base (0.5 M KOH)  
[51:52] Stepping pH = 5.45  
[51:52] Dispensed 0.000635 mL of Base (0.5 M KOH)  
[51:57] Stepping pH = 5.60  
[52:12] Stirrer speed set to 0  
[52:23] Datapoint id 53 collected  
[52:23] Charge balance equation is out by -12.6%  
[52:23] Stirrer speed set to 55  
[52:28] pH 5.65 -> 5.85  
[52:28] Using charge balance adjust  
[52:28] Dispensed 0.000659 mL of Base (0.5 M KOH)  
[52:48] Stirrer speed set to 0  
[53:00] Datapoint id 54 collected  
[53:00] Charge balance equation is out by 0.5%  
[53:00] Stirrer speed set to 55

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[53:05] pH 5.86 -> 6.06  
[53:05] Using charge balance adjust  
[53:06] Dispensed 0.000447 mL of Base (0.5 M KOH)  
[53:26] Stirrer speed set to 0  
[53:39] Datapoint id 55 collected  
[53:39] Charge balance equation is out by -8.3%  
[53:39] Stirrer speed set to 55  
[53:44] pH 6.05 -> 6.25  
[53:44] Using charge balance adjust  
[53:44] Dispensed 0.000329 mL of Base (0.5 M KOH)  
[54:04] Stirrer speed set to 0  
[54:18] Datapoint id 56 collected  
[54:18] Charge balance equation is out by -4.8%  
[54:18] Stirrer speed set to 55  
[54:23] pH 6.24 -> 6.44  
[54:23] Using charge balance adjust  
[54:23] Dispensed 0.000235 mL of Base (0.5 M KOH)  
[54:44] Stirrer speed set to 0  
[55:11] Datapoint id 57 collected  
[55:11] Charge balance equation is out by -4.5%  
[55:11] Stirrer speed set to 55  
[55:16] pH 6.43 -> 6.63  
[55:16] Using charge balance adjust  
[55:16] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[55:37] Stirrer speed set to 0  
[56:04] Datapoint id 58 collected  
[56:04] Charge balance equation is out by -2.3%  
[56:04] Stirrer speed set to 55  
[56:09] pH 6.63 -> 6.83  
[56:09] Using charge balance adjust  
[56:09] Dispensed 0.000118 mL of Base (0.5 M KOH)  
[56:29] Stirrer speed set to 0  
[57:08] Datapoint id 59 collected  
[57:08] Charge balance equation is out by -7.5%  
[57:08] Stirrer speed set to 55  
[57:13] pH 6.81 -> 7.01  
[57:13] Using charge balance adjust  
[57:13] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[57:33] Stirrer speed set to 0  
[58:22] Datapoint id 60 collected  
[58:22] Charge balance equation is out by -25.4%  
[58:22] Stirrer speed set to 55  
[58:28] pH 6.94 -> 7.14  
[58:28] Using cautious pH adjust  
[58:28] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[58:33] Stepping pH = 6.96  
[58:33] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[58:38] Stepping pH = 7.14  
[58:53] Stirrer speed set to 0  
[59:53] Datapoint id 61 collected  
[59:53] Charge balance equation is out by -82.5%  
[59:53] Stirrer speed set to 55  
[59:58] pH 7.28 -> 7.48  
[59:58] Using cautious pH adjust  
[59:58] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:00:03] Stepping pH = 7.34  
[1:00:03] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:00:08] Stepping pH = 7.41  
[1:00:09] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:00:14] Stepping pH = 7.51  
[1:00:29] Stirrer speed set to 0  
[1:01:29] Datapoint id 62 collected  
[1:01:29] Charge balance equation is out by -78.6%  
[1:01:29] Stirrer speed set to 55  
[1:01:34] pH 7.53 -> 7.73  
[1:01:34] Using cautious pH adjust  
[1:01:34] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:01:39] Stepping pH = 7.61  
[1:01:39] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:01:44] Stepping pH = 7.72  
[1:01:59] Stirrer speed set to 0  
[1:02:59] Datapoint id 63 collected  
[1:02:59] Charge balance equation is out by -84.1%  
[1:02:59] Stirrer speed set to 55  
[1:03:04] pH 7.73 -> 7.93  
[1:03:04] Using cautious pH adjust  
[1:03:04] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:03:09] Stepping pH = 7.79  
[1:03:10] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:03:15] Stepping pH = 7.89  
[1:03:15] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:03:20] Stepping pH = 7.99  
[1:03:35] Stirrer speed set to 0  
[1:04:35] Datapoint id 64 collected  
[1:04:35] Charge balance equation is out by -269.2%  
[1:04:35] Stirrer speed set to 55  
[1:04:40] pH 8.03 -> 8.23  
[1:04:40] Using cautious pH adjust  
[1:04:40] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:04:45] Stepping pH = 8.10  
[1:04:45] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:04:50] Stepping pH = 8.18  
[1:04:50] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:04:55] Stepping pH = 8.27  
[1:05:10] Stirrer speed set to 0  
[1:05:35] Datapoint id 65 collected  
[1:05:35] Charge balance equation is out by -326.7%  
[1:05:35] Stirrer speed set to 55  
[1:05:40] pH 8.29 -> 8.49  
[1:05:40] Using cautious pH adjust  
[1:05:40] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:05:45] Stepping pH = 8.32  
[1:05:45] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:05:50] Stepping pH = 8.36  
[1:05:51] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:05:56] Stepping pH = 8.37  
[1:05:56] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:06:01] Stepping pH = 8.53  
[1:06:16] Stirrer speed set to 0  
[1:06:45] Datapoint id 66 collected  
[1:06:45] Charge balance equation is out by -901.8%  
[1:06:45] Stirrer speed set to 55  
[1:06:50] pH 8.59 -> 8.79  
[1:06:50] Using cautious pH adjust  
[1:06:50] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:06:55] Stepping pH = 8.62  
[1:06:55] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:07:00] Stepping pH = 8.66

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:07:00] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:07:05] Stepping pH = 8.73  
[1:07:05] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:07:11] Stepping pH = 8.78  
[1:07:26] Stirrer speed set to 0  
[1:07:42] Datapoint id 67 collected  
[1:07:42] Charge balance equation is out by -378.7%  
[1:07:42] Stirrer speed set to 55  
[1:07:47] pH 8.81 -> 9.01  
[1:07:47] Using cautious pH adjust  
[1:07:47] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:07:52] Stepping pH = 8.81  
[1:07:53] Dispensed 0.000118 mL of Base (0.5 M KOH)  
[1:07:58] Stepping pH = 8.81  
[1:07:58] Dispensed 0.000564 mL of Base (0.5 M KOH)  
[1:08:03] Stepping pH = 9.06  
[1:08:18] Stirrer speed set to 0  
[1:08:32] Datapoint id 68 collected  
[1:08:32] Charge balance equation is out by -1,458.4%  
[1:08:32] Stirrer speed set to 55  
[1:08:37] pH 9.20 -> 9.40  
[1:08:37] Using cautious pH adjust  
[1:08:37] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:08:42] Stepping pH = 9.21  
[1:08:42] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[1:08:47] Stepping pH = 9.28  
[1:08:47] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:08:53] Stepping pH = 9.44  
[1:09:08] Stirrer speed set to 0  
[1:09:26] Datapoint id 69 collected  
[1:09:26] Charge balance equation is out by -266.5%  
[1:09:26] Stirrer speed set to 55  
[1:09:31] pH 9.51 -> 9.71  
[1:09:31] Using cautious pH adjust  
[1:09:31] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:09:36] Stepping pH = 9.51  
[1:09:36] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[1:09:41] Stepping pH = 9.70  
[1:09:56] Stirrer speed set to 0  
[1:10:09] Datapoint id 70 collected  
[1:10:09] Charge balance equation is out by -98.1%  
[1:10:09] Stirrer speed set to 55  
[1:10:14] pH 9.79 -> 9.99  
[1:10:14] Using cautious pH adjust  
[1:10:14] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:10:19] Stepping pH = 9.80  
[1:10:19] Dispensed 0.000447 mL of Base (0.5 M KOH)  
[1:10:24] Stepping pH = 10.04  
[1:10:39] Stirrer speed set to 0  
[1:10:49] Datapoint id 71 collected  
[1:10:49] Charge balance equation is out by -90.6%  
[1:10:49] Titration 3 of 3  
[1:10:49] Adding initial titrants  
[1:10:49] Automatically add 0.30000 mL of Octanol  
[1:10:56] Dispensed 0.300000 mL of Octanol  
[1:10:56] Stirrer speed set to 10  
[1:10:58] Stirrer speed set to 60  
[1:10:58] Iterative adjust 10.07 -> 2.00  
[1:10:58] pH 10.07 -> 2.00



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:11:00] Dispensed 0.100000 mL of Acid (0.5 M HCl)  
[1:11:05] pH 2.05 -> 2.00  
[1:11:05] Dispensed 0.007996 mL of Acid (0.5 M HCl)  
[1:11:56] Stirrer speed set to 0  
[1:12:06] Datapoint id 72 collected  
[1:12:06] Stirrer speed set to 60  
[1:12:11] pH 1.98 -> 2.18  
[1:12:11] Using cautious pH adjust  
[1:12:11] Dispensed 0.015334 mL of Base (0.5 M KOH)  
[1:12:16] Stepping pH = 2.06  
[1:12:17] Dispensed 0.011900 mL of Base (0.5 M KOH)  
[1:12:22] Stepping pH = 2.16  
[1:12:22] Dispensed 0.001834 mL of Base (0.5 M KOH)  
[1:12:27] Stepping pH = 2.18  
[1:12:42] Stirrer speed set to 0  
[1:12:52] Datapoint id 73 collected  
[1:12:52] Charge balance equation is out by 5.2%  
[1:12:52] Stirrer speed set to 60  
[1:12:57] pH 2.19 -> 2.39  
[1:12:57] Using charge balance adjust  
[1:12:58] Dispensed 0.019450 mL of Base (0.5 M KOH)  
[1:13:18] Stirrer speed set to 0  
[1:13:28] Datapoint id 74 collected  
[1:13:28] Charge balance equation is out by 10.4%  
[1:13:28] Stirrer speed set to 60  
[1:13:33] pH 2.42 -> 2.62  
[1:13:33] Using charge balance adjust  
[1:13:34] Dispensed 0.012676 mL of Base (0.5 M KOH)  
[1:13:54] Stirrer speed set to 0  
[1:14:04] Datapoint id 75 collected  
[1:14:04] Charge balance equation is out by 3.9%  
[1:14:04] Stirrer speed set to 60  
[1:14:09] pH 2.63 -> 2.83  
[1:14:09] Using charge balance adjust  
[1:14:09] Dispensed 0.008843 mL of Base (0.5 M KOH)  
[1:14:29] Stirrer speed set to 0  
[1:14:39] Datapoint id 76 collected  
[1:14:39] Charge balance equation is out by 9.8%  
[1:14:39] Stirrer speed set to 60  
[1:14:45] pH 2.86 -> 3.06  
[1:14:45] Using charge balance adjust  
[1:14:45] Dispensed 0.006256 mL of Base (0.5 M KOH)  
[1:15:05] Stirrer speed set to 0  
[1:15:15] Datapoint id 77 collected  
[1:15:15] Charge balance equation is out by -0.7%  
[1:15:15] Stirrer speed set to 60  
[1:15:20] pH 3.06 -> 3.26  
[1:15:20] Using charge balance adjust  
[1:15:20] Dispensed 0.004704 mL of Base (0.5 M KOH)  
[1:15:41] Stirrer speed set to 0  
[1:15:51] Datapoint id 78 collected  
[1:15:51] Charge balance equation is out by 11.5%  
[1:15:51] Stirrer speed set to 60  
[1:15:56] pH 3.28 -> 3.48  
[1:15:56] Using charge balance adjust  
[1:15:56] Dispensed 0.003622 mL of Base (0.5 M KOH)  
[1:16:16] Stirrer speed set to 0  
[1:16:26] Datapoint id 79 collected  
[1:16:26] Charge balance equation is out by 4.3%

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:16:26] Stirrer speed set to 60  
[1:16:31] pH 3.50 -> 3.70  
[1:16:31] Using charge balance adjust  
[1:16:31] Dispensed 0.003057 mL of Base (0.5 M KOH)  
[1:16:52] Stirrer speed set to 0  
[1:17:02] Datapoint id 80 collected  
[1:17:02] Charge balance equation is out by 17.0%  
[1:17:02] Stirrer speed set to 60  
[1:17:07] pH 3.73 -> 3.93  
[1:17:07] Using cautious pH adjust  
[1:17:07] Dispensed 0.001411 mL of Base (0.5 M KOH)  
[1:17:12] Stepping pH = 3.83  
[1:17:12] Dispensed 0.001011 mL of Base (0.5 M KOH)  
[1:17:17] Stepping pH = 3.91  
[1:17:17] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[1:17:22] Stepping pH = 3.93  
[1:17:37] Stirrer speed set to 0  
[1:17:48] Datapoint id 81 collected  
[1:17:48] Charge balance equation is out by 7.0%  
[1:17:48] Stirrer speed set to 60  
[1:17:53] pH 3.92 -> 4.12  
[1:17:53] Using charge balance adjust  
[1:17:53] Dispensed 0.002752 mL of Base (0.5 M KOH)  
[1:18:13] Stirrer speed set to 0  
[1:18:23] Datapoint id 82 collected  
[1:18:23] Charge balance equation is out by 8.4%  
[1:18:23] Stirrer speed set to 60  
[1:18:29] pH 4.14 -> 4.34  
[1:18:29] Using charge balance adjust  
[1:18:29] Dispensed 0.002611 mL of Base (0.5 M KOH)  
[1:18:49] Stirrer speed set to 0  
[1:18:59] Datapoint id 83 collected  
[1:18:59] Charge balance equation is out by 20.8%  
[1:18:59] Stirrer speed set to 60  
[1:19:04] pH 4.38 -> 4.58  
[1:19:04] Using cautious pH adjust  
[1:19:04] Dispensed 0.001152 mL of Base (0.5 M KOH)  
[1:19:09] Stepping pH = 4.47  
[1:19:09] Dispensed 0.000847 mL of Base (0.5 M KOH)  
[1:19:15] Stepping pH = 4.56  
[1:19:15] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[1:19:20] Stepping pH = 4.58  
[1:19:35] Stirrer speed set to 0  
[1:19:45] Datapoint id 84 collected  
[1:19:45] Charge balance equation is out by 7.2%  
[1:19:45] Stirrer speed set to 60  
[1:19:50] pH 4.57 -> 4.77  
[1:19:50] Using charge balance adjust  
[1:19:50] Dispensed 0.001929 mL of Base (0.5 M KOH)  
[1:20:10] Stirrer speed set to 0  
[1:20:20] Datapoint id 85 collected  
[1:20:20] Charge balance equation is out by -8.5%  
[1:20:20] Stirrer speed set to 60  
[1:20:25] pH 4.75 -> 4.95  
[1:20:25] Using charge balance adjust  
[1:20:26] Dispensed 0.001505 mL of Base (0.5 M KOH)  
[1:20:46] Stirrer speed set to 0  
[1:20:56] Datapoint id 86 collected  
[1:20:56] Charge balance equation is out by -4.5%



Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:20:56] Stirrer speed set to 60  
[1:21:01] pH 4.95 -> 5.15  
[1:21:01] Using charge balance adjust  
[1:21:01] Dispensed 0.001129 mL of Base (0.5 M KOH)  
[1:21:22] Stirrer speed set to 0  
[1:21:32] Datapoint id 87 collected  
[1:21:32] Charge balance equation is out by -5.7%  
[1:21:32] Stirrer speed set to 60  
[1:21:37] pH 5.14 -> 5.34  
[1:21:37] Using charge balance adjust  
[1:21:37] Dispensed 0.000800 mL of Base (0.5 M KOH)  
[1:21:58] Stirrer speed set to 0  
[1:22:09] Datapoint id 88 collected  
[1:22:09] Charge balance equation is out by -0.8%  
[1:22:09] Stirrer speed set to 60  
[1:22:14] pH 5.34 -> 5.54  
[1:22:14] Using charge balance adjust  
[1:22:14] Dispensed 0.000541 mL of Base (0.5 M KOH)  
[1:22:34] Stirrer speed set to 0  
[1:22:46] Datapoint id 89 collected  
[1:22:46] Charge balance equation is out by 1.2%  
[1:22:46] Stirrer speed set to 60  
[1:22:51] pH 5.55 -> 5.75  
[1:22:51] Using charge balance adjust  
[1:22:51] Dispensed 0.000376 mL of Base (0.5 M KOH)  
[1:23:11] Stirrer speed set to 0  
[1:23:29] Datapoint id 90 collected  
[1:23:29] Charge balance equation is out by 9.5%  
[1:23:29] Stirrer speed set to 60  
[1:23:34] pH 5.77 -> 5.97  
[1:23:34] Using charge balance adjust  
[1:23:34] Dispensed 0.000259 mL of Base (0.5 M KOH)  
[1:23:54] Stirrer speed set to 0  
[1:24:16] Datapoint id 91 collected  
[1:24:16] Charge balance equation is out by 7.6%  
[1:24:16] Stirrer speed set to 60  
[1:24:22] pH 6.00 -> 6.20  
[1:24:22] Using charge balance adjust  
[1:24:22] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[1:24:42] Stirrer speed set to 0  
[1:25:12] Datapoint id 92 collected  
[1:25:12] Charge balance equation is out by 18.0%  
[1:25:12] Stirrer speed set to 60  
[1:25:18] pH 6.23 -> 6.43  
[1:25:18] Using cautious pH adjust  
[1:25:18] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:25:23] Stepping pH = 6.29  
[1:25:23] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:25:28] Stepping pH = 6.50  
[1:25:43] Stirrer speed set to 0  
[1:26:43] Datapoint id 93 collected  
[1:26:43] Charge balance equation is out by -15.4%  
[1:26:43] Stirrer speed set to 60  
[1:26:48] pH 6.54 -> 6.74  
[1:26:48] Using cautious pH adjust  
[1:26:48] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:26:53] Stepping pH = 6.63  
[1:26:53] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:26:58] Stepping pH = 6.80

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:27:14] Stirrer speed set to 0  
[1:28:14] Datapoint id 94 collected  
[1:28:14] Charge balance equation is out by 12.0%  
[1:28:14] Stirrer speed set to 60  
[1:28:19] pH 6.78 -> 6.98  
[1:28:19] Using charge balance adjust  
[1:28:19] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:28:39] Stirrer speed set to 0  
[1:29:39] Datapoint id 95 collected  
[1:29:39] Charge balance equation is out by -11.1%  
[1:29:39] Stirrer speed set to 60  
[1:29:44] pH 6.97 -> 7.17  
[1:29:44] Using charge balance adjust  
[1:29:44] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:30:04] Stirrer speed set to 0  
[1:30:15] Datapoint id 96 collected  
[1:30:15] Charge balance equation is out by -76.1%  
[1:30:15] Stirrer speed set to 60  
[1:30:20] pH 6.91 -> 7.11  
[1:30:20] Using cautious pH adjust  
[1:30:20] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:30:25] Stepping pH = 6.90  
[1:30:25] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[1:30:30] Stepping pH = 7.91  
[1:30:45] Stirrer speed set to 0  
[1:31:45] Datapoint id 97 collected  
[1:31:45] Charge balance equation is out by -214.0%  
[1:31:45] Stirrer speed set to 60  
[1:31:50] pH 8.09 -> 8.29  
[1:31:50] Using cautious pH adjust  
[1:31:51] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:31:56] Stepping pH = 8.14  
[1:31:56] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:32:01] Stepping pH = 8.14  
[1:32:01] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:32:06] Stepping pH = 8.36  
[1:32:21] Stirrer speed set to 0  
[1:32:45] Datapoint id 98 collected  
[1:32:45] Charge balance equation is out by -580.1%  
[1:32:45] Stirrer speed set to 60  
[1:32:50] pH 8.43 -> 8.63  
[1:32:50] Using cautious pH adjust  
[1:32:50] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:32:55] Stepping pH = 8.45  
[1:32:55] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:33:00] Stepping pH = 8.48  
[1:33:00] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:33:05] Stepping pH = 8.61  
[1:33:05] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:33:10] Stepping pH = 8.68  
[1:33:25] Stirrer speed set to 0  
[1:33:41] Datapoint id 99 collected  
[1:33:41] Charge balance equation is out by -464.7%  
[1:33:41] Stirrer speed set to 60  
[1:33:46] pH 8.69 -> 8.89  
[1:33:46] Using cautious pH adjust  
[1:33:46] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:33:51] Stepping pH = 8.71  
[1:33:51] Dispensed 0.000047 mL of Base (0.5 M KOH)

Sample name: **M15\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01005**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 6:16:08 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:33:56] Stepping pH = 8.77  
[1:33:56] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:34:01] Stepping pH = 8.90  
[1:34:17] Stirrer speed set to 0  
[1:34:31] Datapoint id 100 collected  
[1:34:31] Charge balance equation is out by -252.1%  
[1:34:31] Stirrer speed set to 60  
[1:34:36] pH 8.96 -> 9.16  
[1:34:36] Using cautious pH adjust  
[1:34:36] Dispensed 0.000024 mL of Base (0.5 M KOH)  
[1:34:41] Stepping pH = 8.98  
[1:34:41] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:34:46] Stepping pH = 9.09  
[1:34:46] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:34:52] Stepping pH = 9.18  
[1:35:07] Stirrer speed set to 0  
[1:35:20] Datapoint id 101 collected  
[1:35:20] Charge balance equation is out by -179.3%  
[1:35:20] Stirrer speed set to 60  
[1:35:25] pH 9.23 -> 9.43  
[1:35:25] Using cautious pH adjust  
[1:35:25] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:35:30] Stepping pH = 9.24  
[1:35:30] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:35:35] Stepping pH = 9.36  
[1:35:35] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[1:35:40] Stepping pH = 9.43  
[1:35:55] Stirrer speed set to 0  
[1:36:07] Datapoint id 102 collected  
[1:36:07] Charge balance equation is out by -161.3%  
[1:36:07] Stirrer speed set to 60  
[1:36:12] pH 9.46 -> 9.66  
[1:36:12] Using cautious pH adjust  
[1:36:12] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:36:17] Stepping pH = 9.47  
[1:36:17] Dispensed 0.000259 mL of Base (0.5 M KOH)  
[1:36:22] Stepping pH = 9.67  
[1:36:38] Stirrer speed set to 0  
[1:36:49] Datapoint id 103 collected  
[1:36:49] Charge balance equation is out by -94.3%  
[1:36:49] Stirrer speed set to 60  
[1:36:54] pH 9.73 -> 9.93  
[1:36:54] Using cautious pH adjust  
[1:36:54] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[1:36:59] Stepping pH = 9.76  
[1:36:59] Dispensed 0.000306 mL of Base (0.5 M KOH)  
[1:37:05] Stepping pH = 9.91  
[1:37:05] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:37:10] Stepping pH = 9.95  
[1:37:25] Stirrer speed set to 0  
[1:37:36] Datapoint id 104 collected  
[1:37:36] Charge balance equation is out by -63.7%  
[1:37:36] Stirrer speed set to 60  
[1:37:41] pH 9.97 -> 10.05  
[1:37:41] Using cautious pH adjust  
[1:37:41] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[1:37:46] Stepping pH = 9.98  
[1:37:46] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:37:51] Stepping pH = 10.04



## Experiment Log

Sample name: **M15\_octanol** Experiment start time: **3/1/2018 6:16:08 AM**  
Assay name: **pH-metric high logP** Analyst: **Pion**  
Assay ID: **18C-01005** Instrument ID: **T312060**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01005\_M15\_octanol\_pH-metric high logP.t3r**

### Experiment Log (continued)

[1:38:06] Stirrer speed set to 0  
[1:38:17] Datapoint id 105 collected  
[1:38:17] Charge balance equation is out by -43.3%  
[1:38:17] Argon flow rate set to 0  
[1:38:21] Titrator arm moved over Titration position